Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Palladium-Catalyzed Cascade Reaction of Haloalkynes with Unactivated Alkenes for Assembly of Functionalized Oxetanes

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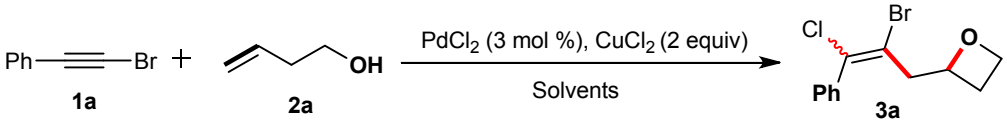
General Information

Melting points were measured using a melting point instrument and are uncorrected. ^{1}H and ^{13}C NMR spectra were recorded on a 400 MHz NMR spectrometer. The chemical shifts are referenced to signals at 7.24 and 77.0 ppm, respectively, and chloroform was used as a solvent with TMS as the internal standard. IR spectra were obtained with an infrared spectrometer on either potassium bromide pellets or liquid films between two potassium bromide pellets. GC-MS data were obtained using electron ionization. HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). TLC was performed using commercially available 100-400 mesh silica gel plates (GF_{254}). Unless otherwise noted, purchased chemicals were used without further purification. The ionic liquids ([Bmim]Cl, $[C_2OHmim]Cl$, and $[C_2O_2mim]Cl$) were synthesized using reported procedures. The bromoalkynes and chloroalkynes were prepared according to the literature.

Typical Procedure for the Preparation of Functionalized Oxetanes

A mixture of haloalkynes (0.15 mmol), enols (0.18 mmol), $PdCl_2$ (1.8 mg, 3 mol%), $AgNO_3$ (0.30 mmol), ionic liquid (0.5 mL) in a test tube (10 mL) equipped with a magnetic stirring bar. The mixture was stirred under the atmosphere of air at room temperature. After the reaction was completed, 10 mL ethyl acetate (3×10 mL) was added into the tube. The combined organic layers were washed with brine to neutral, dried over $MgSO_4$, and concentrated in vacuum. Purification of the residue on a preparative TLC afforded the desired products.

Optimization of the Reaction Solvents[a]



Entry	Solvent	Yield (%)[b]	Z/E
1	[Bmim]Cl	trace	-
2	$[Bmim]BF_4$	N.D.	-
3	$[Bmim]PF_6$	N.D.	-

4	$[C_2OHmim]Cl$	6	95/5
5	[BuPy]Cl	trace	-
6	$[C_2O_2mim]Cl$	9	97/3
7	$[HO_2Etmim]NTf_2$	N.D.	-
8	$[HO_2Etmim]HSO_4$	N.D.	-
9	[CPmim]Cl	8	95/5

[a] Reactions were performed with **1a** (0.15 mmol), **2a** (0.18 mmol), $PdCl_2$ (3 mol %) and $CuCl_2•2H_2O$ (0.3 mmol) in the indicated solvent (0.5 mL) at room temperature for 12 h.

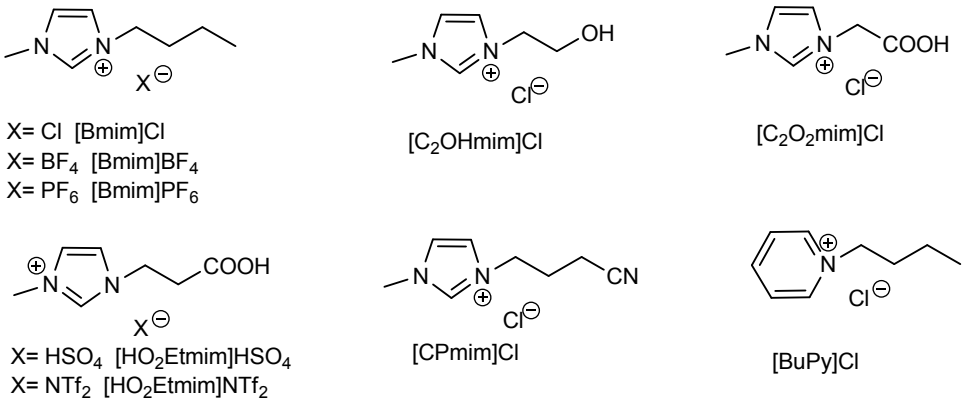
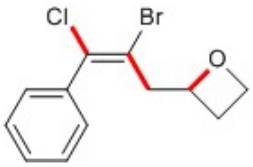


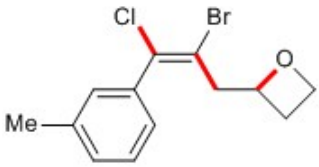
Figure 1. Ionic liquids applied in this work

Characterization Data for All Products



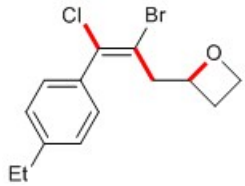
(Z)-2-(2-bromo-3-chloro-3-phenylallyl)oxetane (3a)

Yield: 76% (32.6 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35-7.28 (m, 3H), 7.27-7.21 (m, 2H), 3.86 (dd, J = 13.2, 6.8 Hz, 1H), 3.75-3.61 (m, 3H), 3.22-3.13 (m, 1H), 2.06 (dt, J = 15.6, 7.6 Hz, 1H), 1.87 (dt, J = 12.8, 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.5, 132.5, 129.2, 128.8, 128.6, 128.5, 71.9, 68.6, 44.8, 32.6 ppm; ν_{max}(KBr)/cm^{-1} 3077, 2926, 1641, 1507, 1451, 1410, 1122; MS (EI) m/z 115, 142, 177, 221, 256, 286; HRMS(ESI): m/z calcd for $C_{12}H_{12}BrClNaO$ $[M + Na]^+$ 308.9652, found 308.9652.



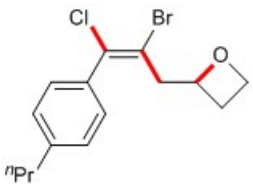
(Z)-2-(2-bromo-3-chloro-3-(*m*-tolyl)allyl)oxetane (3b)

Yield: 78% (35.1 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29 (d, J = 7.6 Hz, 1H), 7.19 (d, J = 7.6 Hz, 1H), 7.13-7.05 (m, 2H), 3.93 (dd, J = 13.2, 8.0 Hz, 1H), 3.81-3.69 (m, 3H), 3.33-3.18 (m, 1H), 2.37 (s, 3H), 2.18-2.07 (m, 1H), 1.93 (dt, J = 12.4, 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 137.5, 132.6, 129.9, 129.1, 128.6, 128.2, 125.6, 72.0, 68.6, 44.8, 32.6, 21.4 ppm; ν_{max}(KBr)/cm^{-1} 3068, 2924, 1635, 1455, 1408, 1110; MS (EI) m/z 115, 128, 153, 176, 190, 254, 300; HRMS(ESI): m/z calcd for $C_{13}H_{14}BrClNaO$ $[M + Na]^+$ 322.9809, found 322.9807.



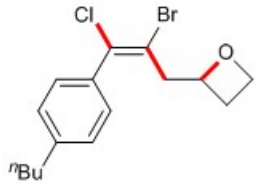
(Z)-2-(2-bromo-3-chloro-3-(4-ethylphenyl)allyl)oxetane (3c)

Yield: 83% (39.1 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22-7.17 (m, 4H), 3.93 (dd, J = 13.2, 8.8 Hz, 1H), 3.82-3.71 (m, 3H), 3.38-3.15 (m, 1H), 2.67 (dd, J = 15.2, 7.6 Hz, 2H), 2.18 -2.09 (m, 1H), 1.95 (dt, J = 12.4, 8.0 Hz, 1H), 1.26 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.5, 134.8, 132.7, 128.5, 128.2, 126.5, 71.9, 68.6, 44.8, 32.6, 28.6, 15.2 ppm; ν_{max}(KBr)/cm^{-1} 3060, 2926, 1642, 1508, 1456, 1109; MS (EI) m/z 115, 141, 153, 191, 204, 268, 283, 314; HRMS(ESI): m/z calcd for $C_{14}H_{16}BrClNaO$ $[M + Na]^+$ 336.9965, found 336.9959.



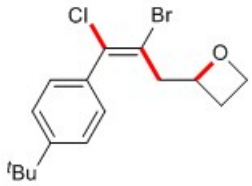
(Z)-2-(2-bromo-3-chloro-3-(4-propylphenyl)allyl)oxetane (3d)

Yield: 77% (37.9 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.16 (m, 4H), 3.92 (dd, J = 13.2, 8.0 Hz, 1H), 3.82-3.69 (m, 3H), 3.32-3.24 (m, 1H), 2.60 (t, J = 7.6 Hz, 2H), 2.18-2.08 (m, 1H), 1.94 (dt, J = 12.8, 8.0 Hz, 1H), 1.66 (q, J = 7.2 Hz, 2H), 0.96 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.0, 134.8, 132.7, 128.8, 128.4, 128.1, 71.9, 68.6, 44.8, 37.8, 32.6, 24.3, 13.9 ppm; ν_{max}(KBr)/cm^{-1} 3062, 2927, 1642, 1505, 1453, 1108; MS (EI) m/z 115, 141, 155, 184, 231, 263, 300, 328; HRMS(ESI): m/z calcd for $C_{15}H_{18}BrClNaO$ $[M + Na]^+$ 351.0122, found 351.0123.



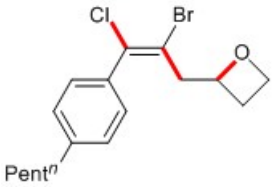
(Z)-2-(2-bromo-3-(4-butylphenyl)-3-chloroallyl)oxetane (3e)

Yield: 79% (40.5 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22-7.16 (m, 4H), 3.92 (dd, J = 13.2, 8.4 Hz, 1H), 3.82-3.69 (m, 3H), 3.32-3.24 (m, 1H), 2.63 (t, J = 7.6 Hz, 2H), 2.19-2.09 (m, 1H), 1.94 (dt, J = 12.8, 8.0 Hz, 1H), 1.62 (dd, J = 14.8, 7.6 Hz, 2H), 1.37 (dt, J = 14.4, 7.2 Hz, 2H), 0.94 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 134.8, 132.8, 128.7, 128.4, 128.1, 71.9, 68.6, 44.7, 35.4, 33.4, 32.6, 22.4, 13.9 ppm; ν_{max}(KBr)/cm^{-1} 3056, 2928, 1642, 1486, 1453, 1102; MS (EI) m/z 115, 141, 176, 198, 245, 277, 342; HRMS(ESI): m/z calcd for $C_{16}H_{20}BrClNaO$ $[M + Na]^+$ 365.0278, found 365.0274.



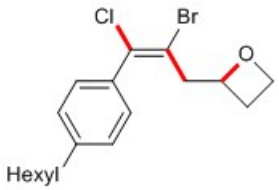
(Z)-2-(2-bromo-3-(4-(tert-butyl)phenyl)-3-chloroallyl)oxetane (3f)

Yield: 85% (43.6 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, J = 7.6 Hz, 2H), 7.23 (d, J = 8.0 Hz, 2H), 3.93 (dd, J = 13.2, 7.6 Hz, 1H), 3.81-3.74 (m, 3H), 3.33-3.25 (m, 1H), 2.18-2.09 (m, 1H), 1.96 (dt, J = 12.4, 8.0 Hz, 1H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 134.5, 132.7, 128.3, 128.1, 125.7, 72.0, 68.6, 44.7, 34.8, 32.6, 31.2 ppm; ν_{max}(KBr)/cm^{-1} 3060, 2927, 1642, 1516, 1464, 1410, 1104; MS (EI) m/z 77, 95, 115, 141, 183, 277, 327, 342; HRMS(ESI): m/z calcd for $C_{16}H_{20}BrClNaO$ $[M + Na]^+$ 365.0278, found 365.0274.



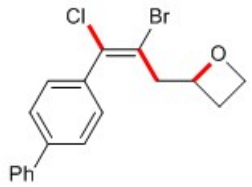
(Z)-2-(2-bromo-3-chloro-3-(4-pentylphenyl)allyl)oxetane (3g)

Yield: 74% (39.5 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23-7.14 (m, 4H), 3.92 (dd, J = 13.2, 8.4 Hz, 1H), 3.82-3.69 (m, 3H), 3.32-3.21 (m, 1H), 2.62 (t, J = 7.6 Hz, 2H), 2.19-2.07 (m, 1H), 1.94 (dt, J = 12.8, 8.0 Hz, 1H), 1.66-1.59 (m, 2H), 1.36-1.30 (m, 4H), 0.90 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 134.8, 132.7, 128.7, 128.4, 128.1, 72.0, 68.6, 44.7, 35.7, 32.6, 31.5, 30.9, 22.5, 14.0 ppm; ν_{max}(KBr)/cm^{-1} 3063, 2928, 1639, 1515, 1465, 1433, 1120; MS (EI) m/z 115, 141, 155, 176, 212, 259, 323, 356; HRMS(ESI): m/z calcd for $C_{17}H_{22}BrClNaO$ $[M + Na]^+$ 379.0435, found 379.0433.



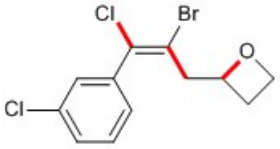
(Z)-2-(2-bromo-3-chloro-3-(4-hexylphenyl)allyl)oxetane (3h)

Yield: 72% (39.9 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22-7.18 (m, 4H), 3.92 (dd, J = 13.2, 8.4 Hz, 1H), 3.82-3.71 (m, 3H), 3.32-3.24 (m, 1H), 2.62 (t, J = 7.6 Hz, 2H), 2.18-2.08 (m, 1H),1.94 (dt, J = 12.8, 8.0 Hz, 1H), 1.66-1.58 (m, 2H), 1.35-1.28 (m, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 134.8, 132.7, 128.7, 128.5, 128.1, 71.9, 68.6, 44.8, 35.8, 32.6, 31.7, 31.2, 29.0, 22.6, 14.1 ppm; ν_{max}(KBr)/cm^{-1} 3057, 2926, 1637, 1485, 1410, 1108; MS (EI) m/z 85, 115, 141, 176, 226, 305, 335, 370; HRMS(ESI): m/z calcd for $C_{18}H_{24}BrClNaO$ $[M + Na]^+$ 393.0591, found 393.0589.



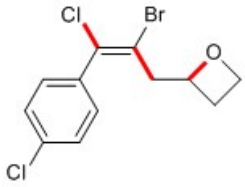
(Z)-2-(3-([1,1'-biphenyl]-4-yl)-2-bromo-3-chloroallyl)oxetane (3i)

Yield: 78% (42.3 mg) as a yellow solid; mp =140.5-141.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67-7.58 (m, 5H), 7.46 (t, J = 7.2 Hz, 2H), 7.38 (d, J = 7.6 Hz, 2H), 3.95 (dd, J = 13.6, 7.6 Hz, 1H), 3.86-3.71 (m, 3H), 3.38-3.30 (m, 1H), 2.21-2.11 (m, 1H), 1.99 (dt, J = 13.2, 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.1, 140.1, 136.3, 132.3, 129.0, 128.9, 128.7, 127.9, 127.4, 127.1, 72.0, 68.6, 44.8, 32.7 ppm; ν_{max}(KBr)/cm^{-1} 3054, 2926, 1643, 1508, 1454, 1414, 1110; MS (EI) m/z 108, 165, 189, 218, 265, 299, 329, 345, 362; HRMS(ESI): m/z calcd for $C_{18}H_{16}BrClNaO$ $[M + Na]^+$ 384.9965, found 384.9967.



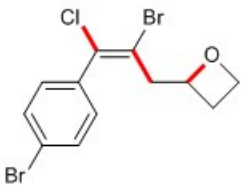
(Z)-2-(2-bromo-3-chloro-3-(3-chlorophenyl)allyl)oxetane (3j)

Yield: 70% (33.6 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.38 (m, 1H), 7.36-7.31 (m, 2H), 7.18 (d, J = 7.2 Hz, 1H), 3.94 (dd, J = 13.2, 8.0 Hz, 1H), 3.82-3.72 (m, 3H), 3.25-3.15 (m, 1H), 2.13 (dt, J = 15.2, 7.6 Hz, 1H), 1.96 (dt, J = 12.4, 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.1, 134.7, 131.0, 130.8, 130.0, 129.4, 128.7, 126.7, 71.9, 68.6, 44.8, 32.6 ppm; ν_{max}(KBr)/cm^{-1} 3056, 2925, 1645, 1519, 1455, 1106; MS (EI) m/z 115, 141, 196, 257, 292, 320; HRMS(ESI): m/z calcd for $C_{12}H_{11}BrCl_2NaO$ $[M + Na]^+$ 342.9263, found 342.9265.



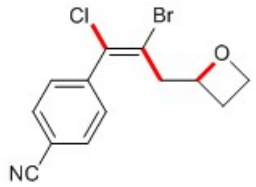
(Z)-2-(2-bromo-3-chloro-3-(4-chlorophenyl)allyl)oxetane (3k)

Yield: 71% (34.1 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 8.0 Hz, 2H), 7.19 (d, J = 8.0 Hz, 2H), 3.92 (dd, J = 13.6, 8.0 Hz, 1H), 3.83-3.71 (m, 3H), 3.36-3.28 (m, 1H), 2.15 (dt, J = 15.2, 7.6 Hz, 1H), 1.96 (dt, J = 12.4, 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.9, 134.5, 132.8, 132.0, 130.4, 123.5, 70.9, 68.6, 43.6, 31.4 ppm; ν_{max}(KBr)/cm^{-1} 3026, 2928, 1641, 1494, 1455, 1112; MS (EI) m/z 105, 139, 176, 220, 255, 281, 320; HRMS(ESI): m/z calcd for $C_{12}H_{11}BrCl_2NaO$ $[M + Na]^+$ 342.9263, found 342.9265.



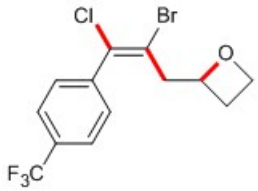
(Z)-2-(2-bromo-3-(4-bromophenyl)-3-chloroallyl)oxetane (3l)

Yield: 70% (38.2 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 7.2 Hz, 2H), 7.18 (d, J = 7.6 Hz, 2H), 3.93 (dd, J = 13.2, 7.2 Hz, 1H), 3.80-3.70 (m, 3H), 3.25-3.16 (m, 1H), 2.13 (dt, J = 16.0, 8.4 Hz, 1H), 1.96 (dt, J = 12.4, 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 132.0, 131.2, 130.2, 129.2, 123.5, 71.9, 68.5, 44.8, 32.6 ppm; ν_{max}(KBr)/cm^{-1} 3050, 2924, 1645, 1516, 1462, 1412, 1109; MS (EI) m/z 115, 141, 176, 220, 277, 301, 364; HRMS(ESI): m/z calcd for $C_{12}H_{11}Br_2ClNaO$ $[M + Na]^+$ 386.8757, found 386.8753.



(Z)-4-(2-bromo-1-chloro-3-(oxetan-2-yl)prop-1-en-1-yl)benzonitrile (3m)

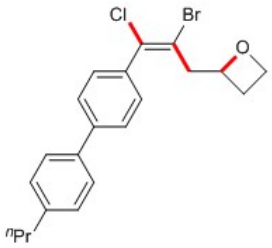
Yield: 63% (29.4 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, J = 7.6 Hz, 2H), 7.44 (d, J = 7.6 Hz, 2H), 3.95 (dd, J = 13.6, 8.2 Hz, 1H), 3.76 (dq, J = 16.4, 8.0 Hz, 3H), 3.14 (p, J = 7.6 Hz, 1H), 2.13 (dt, J = 16.0, 8.4 Hz, 1H), 1.95 (dt, J = 12.4, 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.8, 132.6, 132.2, 130.2, 129.5, 117.9, 113.2, 71.9, 68.5, 44.9, 32.7 ppm; ν_{max}(KBr)/cm^{-1} 3045, 2925, 2262, 1641, 1498, 1415, 1127; MS (EI) m/z 140, 167, 202, 248, 283, 311; HRMS(ESI): m/z calcd for $C_{13}H_{11}BrClNNaO$ $[M + Na]^+$ 333.9605, found 333.9603.



(Z)-2-(2-bromo-3-chloro-3-(4-(trifluoromethyl)phenyl)allyl)oxetane (3n)

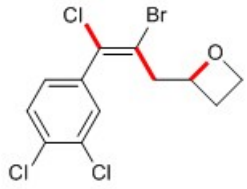
Yield: 64% (34.0 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, J = 8.0 Hz, 2H), 7.44 (d, J = 8.0 Hz, 2H), 3.94 (dd, J = 13.2, 8.4 Hz, 1H), 3.82-3.70 (m, 3H), 3.23-3.11 (m, 1H), 2.14 (td, J = 15.2, 7.6 Hz, 1H), 2.01-1.92 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.0, 131.3 (q,

J = 1.6 Hz), 130.7, 129.9 (q, J = 32.8 Hz), 125.8 (q, J = 3.7 Hz), 125.3 (q, J = 269.8 Hz), 71.9, 68.5, 44.8, 32.6 ppm; ν_{max}(KBr)/cm^{-1} 3038, 2928, 1643, 1484, 1454, 1109; MS (EI) m/z 115, 141, 183, 210, 245, 289, 326, 354; HRMS(ESI): m/z calcd for $C_{13}H_{11}BrClF_3NaO$ $[M + Na]^+$ 376.9526, found 376.9522.



(Z)-2-(2-bromo-3-chloro-3-(4'-propyl-[1,1'-biphenyl]-4-yl)allyl)oxetane (3o)

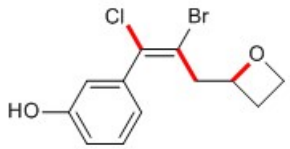
Yield: 78% (47.3 mg) as a yellow solid; mp =147.3-148.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 7.2 Hz, 2H), 7.51 (d, J = 7.2 Hz, 2H), 7.36 (d, J = 7.2 Hz, 2H), 7.27 (d, J = 8.4 Hz, 2H), 3.95 (dd, J = 14.4, 7.6 Hz, 1H), 3.86-3.70 (m, 3H), 3.40-3.27 (m, 1H), 2.64 (t, J = 6.8 Hz, 2H), 2.16 (dq, J = 15.6, 7.6 Hz, 1H), 2.07-1.90 (m, 1H), 1.69 (dd, J = 14.4, 7.2 Hz, 2H), 0.98 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.6, 142.1, 137.4, 136.0, 132.4, 129.0, 128.9, 128.6, 127.2, 127.0, 72.0, 68.6, 44.8, 37.7, 32.7, 24.5, 13.8 ppm; ν_{max}(KBr)/cm^{-1} 3058, 2928, 1642, 1482, 1415, 1121; MS (EI) m/z 115, 139, 207, 231, 281, 307, 339, 369, 404; HRMS(ESI): m/z calcd for $C_{21}H_{22}BrClNaO$ $[M + Na]^+$ 427.0435, found 427.0431.



(Z)-2-(2-bromo-3-chloro-3-(3,4-dichlorophenyl)allyl)oxetane (3p)

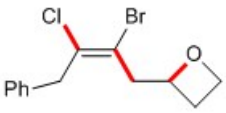
Yield: 72% (38.2 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (d, J = 8.0 Hz, 1H), 7.42 (s, 1H), 7.14 (d, J = 8.4 Hz, 1H), 3.94 (dd, J = 13.2, 8.4 Hz, 1H), 3.77 (dt, J = 15.6, 8.6 Hz,

3H), 3.26-3.13 (m, 1H), 2.13 (dq, J = 15.2, 7.6 Hz, 1H), 1.96 (dt, J = 12.8, 7.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.2, 133.7, 133.1, 130.8, 130.6, 130.2, 129.8, 127.9, 71.9, 68.6, 44.8, 32.6 ppm; ν_{max}(KBr)/cm^{-1} 3027, 2927, 1642, 1495, 1457, 1111; MS (EI) m/z 139, 175, 210, 245, 289, 326, 354; HRMS(ESI): m/z calcd for $C_{12}H_{10}BrCl_3NaO$ $[M + Na]^+$ 376.8873, found 376.8871.



(Z)-3-(2-bromo-1-chloro-3-(oxetan-2-yl)prop-1-en-1-yl)phenol (3q)

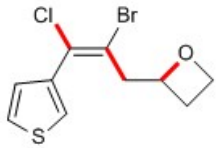
Yield: 54% (24.5 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27 (d, J = 5.6 Hz, 1H), 6.85 (d, J = 8.2 Hz, 2H), 6.79 (s, 1H), 4.16-4.07 (m, 1H), 3.94 (dd, J = 13.2, 8.4 Hz, 1H), 3.84-3.70 (m, 2H), 3.36-3.24 (m, 1H), 2.13 (dt, J = 20.0, 7.6 Hz, 1H), 2.01-1.90 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.8, 138.9, 131.9, 130.0, 128.6, 120.9, 116.3, 115.5, 71.9, 68.6, 44.8, 32.6 ppm; ν_{max}(KBr)/cm^{-1} 3027, 2928, 1642, 1484, 1453, 1124; MS (EI) m/z 119, 147, 182, 228, 293, 302; HRMS(ESI): m/z calcd for $C_{12}H_{12}BrClNaO_2$ $[M + Na]^+$ 324.9601, found 324.9595.



(Z)-2-(2-bromo-3-chloro-4-phenylbut-2-en-1-yl)oxetane (3r)

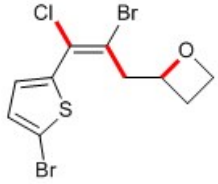
Yield: 70% (31.5 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (t, J = 7.2 Hz, 2H), 7.27 (d, J = 10.8 Hz, 1H), 7.19 (d, J = 7.2 Hz, 2H), 3.96 (dd, J = 13.2, 8.4 Hz, 1H), 3.91-3.78 (m, 4H), 3.73 (dd, J = 15.6, 7.6 Hz, 1H), 3.57 (dt, J = 16.0, 8.0 Hz, 1H), 2.19-2.10 (m, 1H), 2.09-1.99 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 133.0, 128.8, 128.1, 127.3, 127.1, 71.8, 68.5, 44.0, 42.0, 32.4 ppm; ν_{max}(KBr)/cm^{-1} 3038, 2926, 1645, 1500, 1455, 1111; MS (EI) m/z 91, 115, 128,

155, 185, 221, 264, 300; HRMS(ESI): m/z calcd for $C_{13}H_{14}BrClNaO$ $[M + Na]^+$ 322.9809, found 322.9806.



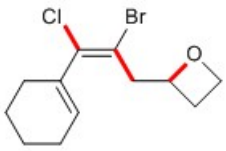
(Z)-2-(2-bromo-3-chloro-3-(thiophen-3-yl)allyl)oxetane (3s)

Yield: 61% (26.7 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 4.8 Hz, 1H), 7.31 (s, 1H), 7.09 (d, J = 4.8 Hz, 1H), 3.95 (dd, J = 13.2, 8.0 Hz, 1H), 3.85-3.73 (m, 3H), 3.50-3.39 (m, 1H), 2.14 (dq, J = 15.2, 7.6 Hz, 1H), 1.98 (dt, J = 20.0, 10.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.2, 129.2, 127.7, 127.4, 126.3, 125.2, 72.1, 68.6, 44.8, 32.7 ppm; ν_{max}(KBr)/cm^{-1} 3037, 2926, 1643, 1456, 1412, 1127; MS (EI) m/z 115, 134, 168, 213, 246, 292; HRMS(ESI): m/z calcd for $C_{10}H_{10}BrClNaOS$ $[M + Na]^+$ 314.9216, found 314.9215.



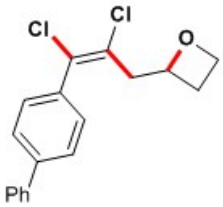
(Z)-2-(2-bromo-3-(5-bromothiophen-2-yl)-3-chloroallyl)oxetane (3t)

Yield: 59% (32.7 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.97 (d, J = 3.6 Hz, 1H), 6.85 (d, J = 3.6 Hz, 1H), 3.96 (dd, J = 13.2, 8.0 Hz, 1H), 3.85 (t, J = 8.4 Hz, 1H), 3.76 (dd, J = 16.4, 8.4 Hz, 2H), 3.64-3.46 (m, 1H), 2.14 (td, J = 15.2, 8.0 Hz, 1H), 2.06-1.96 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.6, 132.2, 129.8, 128.9, 124.5, 115.2, 72.2, 68.6, 45.1, 33.0 ppm; ν_{max}(KBr)/cm^{-1} 3037, 2927, 1643, 1454, 1410, 1121; MS (EI) m/z 119, 147, 182, 228, 263, 305, 370; HRMS(ESI): m/z calcd for $C_{10}H_9Br_2ClNaOS$ $[M + Na]^+$ 392.8322, found 392.8317.



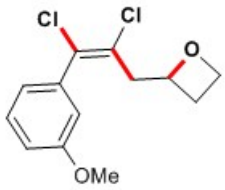
(Z)-2-(2-bromo-3-chloro-3-(cyclohex-1-en-1-yl)allyl)oxetane (3u)

Yield: 63% (27.4 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.75 (s, 1H), 3.93 (dd, J = 13.6, 8.2 Hz, 1H), 3.86-3.78 (m, 2H), 3.68 (t, J = 8.4 Hz, 1H), 3.59-3.48 (m, 1H), 2.12 (dd, J = 12.0, 6.8 Hz, 4H), 2.05-1.91 (m, 2H), 1.69 (dd, J = 11.2, 5.6 Hz, 2H), 1.65-1.59 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.8, 135.5, 130.1, 126.5, 72.1, 68.6, 44.6, 32.6, 27.3, 25.3, 22.3, 21.6 ppm; ν_{max}(KBr)/cm^{-1} 3057, 2927, 1642, 1452, 1413, 1120; MS (EI) m/z 77, 91, 105, 145, 175, 211, 253, 290; HRMS(ESI): m/z calcd for $C_{12}H_{16}BrClNaO$ $[M + Na]^+$ 312.9965, found 312.9963.



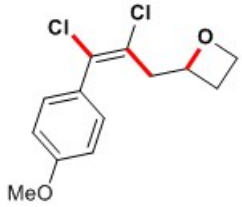
(Z)-2-(3-([1,1'-biphenyl]-4-yl)-2,3-dichloroallyl)oxetane (5a)

Yield: 67% (31.9 mg) as a yellow solid; mp =112.3-113.8 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (t, J = 8.4 Hz, 4H), 7.46 (t, J = 7.6 Hz, 2H), 7.39 (d, J = 8.0 Hz, 3H), 3.94 (dd, J = 13.6, 8.0 Hz, 1H), 3.87 (t, J = 8.4 Hz, 1H), 3.83 - 3.72 (m, 2H), 3.45 (p, J = 8.0 Hz, 1H), 2.19 (dq, J = 15.2, 7.6 Hz, 1H), 2.04-1.95 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.2, 140.1, 135.9, 133.9, 129.5, 129.3, 128.9, 127.9, 127.4, 127.1, 71.0, 68.7, 43.6, 31.5 ppm; ν_{max}(KBr)/cm^{-1} 3050, 2925, 1644, 1515, 1456, 1111; MS (EI) m/z 108, 126, 165, 189, 217, 253, 283, 318; HRMS(ESI): m/z calcd for $C_{18}H_{16}Cl_2NaO$ $[M + Na]^+$ 341.0470, found 341.0468.



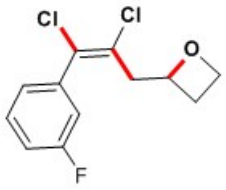
(Z)-2-(2,3-dichloro-3-(3-methoxyphenyl)allyl)oxetane (5b)

Yield: 56% (22.8 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (t, J = 8.0 Hz, 1H), 6.90 (dd, J = 15.2, 8.0 Hz, 2H), 6.84 (s, 1H), 3.92 (dd, J = 13.6, 8.2 Hz, 1H), 3.82 (s, 3H), 3.75 (td, J = 16.0, 8.0 Hz, 3H), 3.39 (p, J = 8.0 Hz, 1H), 2.16 (dq, J = 15.2, 7.6 Hz, 1H), 2.05-1.84 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.6, 138.2, 133.8, 129.8, 129.4, 121.1, 114.8, 114.4, 71.0, 68.7, 55.4, 43.6, 31.4 ppm; ν_{max}(KBr)/cm^{-1} 3046, 2927, 1642, 1511, 1454, 1133; MS (EI) m/z 102, 128, 172, 207, 227, 272; HRMS(ESI): m/z calcd for $C_{13}H_{14}Cl_2NaO_2$ $[M + Na]^+$ 295.0263, found 295.0260.



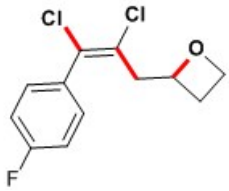
(Z)-2-(2,3-dichloro-3-(4-methoxyphenyl)allyl)oxetane (5c)

Yield: 62% (25.3 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, J = 11.2 Hz, 2H), 6.91 (d, J = 8.6 Hz, 2H), 3.95-3.89 (m, 1H), 3.83 (s, 1H), 3.82-3.70 (m, 3H), 3.46-3.31 (m, 1H), 2.17 (tt, J = 15.2, 7.6 Hz, 1H), 2.01-1.87 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 133.1, 130.6, 130.2, 129.3, 114.1, 71.0, 68.7, 55.4, 43.6, 31.4 ppm; ν_{max}(KBr)/cm^{-1} 3047, 2926, 1643, 1513, 1455, 1135; MS (EI) m/z 105, 128, 167, 183, 207, 237, 272; HRMS(ESI): m/z calcd for $C_{13}H_{14}Cl_2NaO_2$ $[M + Na]^+$ 295.0263, found 295.0263.



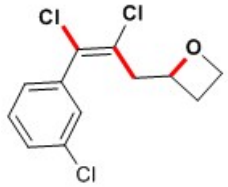
(Z)-2-(2,3-dichloro-3-(3-fluorophenyl)allyl)oxetane (5d)

Yield: 67% (26.1 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (dd, J = 14.0, 7.6 Hz, 1H), 7.10 (t, J = 7.0 Hz, 2H), 7.04 (d, J = 9.0 Hz, 1H), 3.93 (dd, J = 13.6, 8.2 Hz, 1H), 3.88-3.70 (m, 3H), 3.40-3.28 (m, 1H), 2.16 (td, J = 15.2, 7.6 Hz, 1H), 2.03-1.93 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.5 (d, J = 248.4 Hz), 138.9 (d, J = 7.9 Hz), 134.7, 130.4 (d, J = 8.4 Hz), 128.1 (d, J = 2.1 Hz), 124.6 (d, J = 3.1 Hz), 116.2 (d, J = 50.1 Hz), 116.1 (d, J = 6.9 Hz), 70.9, 68.6, 43.6, 31.4 ppm; ν_{max}(KBr)/cm^{-1} 3047, 2926, 1644, 1513, 1455, 1117; MS (EI) m/z 133, 146, 159, 180, 195, 230, 260; HRMS(ESI): m/z calcd for $C_{12}H_{11}Cl_2FNaO$ $[M + Na]^+$ 283.0063, found 283.0064.



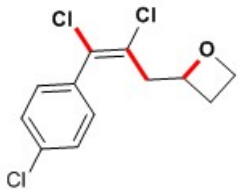
(Z)-2-(2,3-dichloro-3-(4-fluorophenyl)allyl)oxetane (5e)

Yield: 68% (26.5 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.27 (m, 2H), 7.09 (t, J = 8.4 Hz, 2H), 3.92 (dd, J = 13.2, 8.4 Hz, 1H), 3.85-3.69 (m, 3H), 3.39-3.24 (m, 1H), 2.16 (td, J = 15.2, 7.6 Hz, 1H), 2.01-1.91 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 182.0, 162.9 (d, J = 248.7 Hz), 134.2, 133.1 (d, J = 3.6 Hz), 131.0 (d, J = 8.4 Hz), 116.0 (d, J = 21.9 Hz), 70.9, 68.6, 43.6, 31.4 ppm; ν_{max}(KBr)/cm^{-1} 3048, 2925, 1640, 1515, 1430, 1134; MS (EI) m/z 133, 159, 180, 195, 230, 260; HRMS(ESI): m/z calcd for $C_{12}H_{11}Cl_2FNaO$ $[M + Na]^+$ 283.0063, found 283.0063.



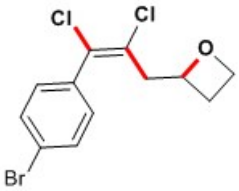
(Z)-2-(2,3-dichloro-3-(3-chlorophenyl)allyl)oxetane (5f)

Yield: 69% (28.6 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.30 (m, 3H), 7.19 (d, J = 7.2 Hz, 1H), 3.93 (dd, J = 13.6, 8.0 Hz, 1H), 3.83 (t, J = 8.4 Hz, 1H), 3.75 (dd, J = 15.6, 8.4 Hz, 2H), 3.32 (p, J = 8.0 Hz, 1H), 2.16 (dq, J = 15.2, 7.6 Hz, 1H), 2.05-1.93 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.6, 134.9, 134.7, 130.0, 129.4, 129.0, 128.1, 127.0, 71.0, 68.7, 43.6, 31.4 ppm; ν_{max}(KBr)/cm^{-1} 3057, 2927, 1644, 1514, 1432, 1108; MS (EI) m/z 113, 141, 176, 196, 211, 246, 276; HRMS(ESI): m/z calcd for $C_{12}H_{11}Cl_3NaO$ $[M + Na]^+$ 298.9768, found 298.9764.



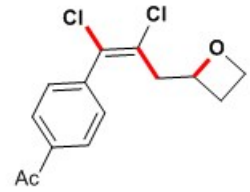
(Z)-2-(2,3-dichloro-3-(4-chlorophenyl)allyl)oxetane (5g)

Yield: 68% (28.2 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 (d, J = 8.4 Hz, 2H), 7.25 (d, J = 7.0 Hz, 2H), 3.92 (dd, J = 13.6, 8.0 Hz, 1H), 3.86-3.68 (m, 3H), 3.39-3.26 (m, 1H), 2.16 (td, J = 15.2, 7.6 Hz, 1H), 2.02-1.89 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.4, 135.3, 134.5, 130.2, 129.1, 128.4, 71.0, 68.6, 43.6, 31.4 ppm; ν_{max}(KBr)/cm^{-1} 3037, 2928, 1644, 1515, 1445, 1133; MS (EI) m/z 105, 128, 171, 190, 203, 233, 276; HRMS(ESI): m/z calcd for $C_{12}H_{11}Cl_3NaO$ $[M + Na]^+$ 298.9768, found 298.9766.



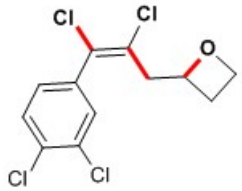
(Z)-2-(3-(4-bromophenyl)-2,3-dichloroallyl)oxetane (5h)

Yield: 68% (32.6 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 8.4 Hz, 2H), 7.19 (d, J = 8.4 Hz, 2H), 3.92 (dd, J = 13.8, 8.2 Hz, 1H), 3.85-3.69 (m, 3H), 3.32 (p, J = 8.0 Hz, 1H), 2.15 (dq, J = 15.2, 7.6 Hz, 1H), 1.96 (dt, J = 12.4, 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.9, 134.5, 132.0, 130.5, 128.4, 123.6, 71.0, 68.6, 43.6, 31.4 ppm; ν_{max}(KBr)/cm^{-1} 3056, 2925, 1645, 1516, 1437, 1132; MS (EI) m/z 113, 127, 141, 175, 196, 211, 255, 290, 320; HRMS(ESI): m/z calcd for $C_{12}H_{11}BrCl_2NaO$ $[M + Na]^+$ 342.9263, found 342.9259.



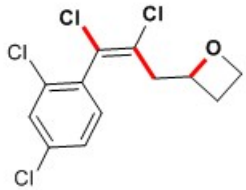
(Z)-1-(4-(1,2-dichloro-3-(oxetan-2-yl)prop-1-en-1-yl)phenyl)ethanone (5i)

Yield: 57% (24.3 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 8.0 Hz, 2H), 7.43 (d, J = 8.0 Hz, 1H), 7.31 (d, J = 8.0 Hz, 1H), 3.97-3.89 (m, 1H), 3.88-3.56 (m, 3H), 3.40-3.13 (m, 1H), 2.62 (s, 3H), 2.25-2.06 (m, 1H), 2.03-1.76 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.6, 142.6, 141.4, 129.2, 128.7, 128.5, 115.7, 71.4, 67.9, 45.7, 31.0, 26.7 ppm; ν_{max}(KBr)/cm^{-1} 3047, 2926, 1645, 1515, 1446, 1115; MS (EI) m/z 115, 141, 176, 219, 239, 254, 284; HRMS(ESI): m/z calcd for $C_{14}H_{14}Cl_2NaO_2$ $[M + Na]^+$ 307.0263, found 307.0265.



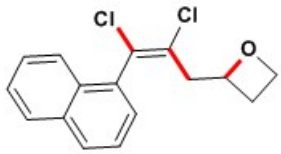
(Z)-2-(2,3-dichloro-3-(3,4-dichlorophenyl)allyl)oxetane (5j)

Yield: 73% (33.9 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, J = 8.4 Hz, 1H), 7.43 (s, 1H), 7.15 (d, J = 8.0 Hz, 1H), 3.93 (dd, J = 13.6, 8.2 Hz, 1H), 3.83 (t, J = 8.4 Hz, 1H), 3.76 (dd, J = 16.4, 8.4 Hz, 2H), 3.43-3.24 (m, 1H), 2.16 (td, J = 15.2, 7.6 Hz, 1H), 2.07-1.91 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.7, 135.5, 133.7, 133.1, 130.8, 130.7, 128.1, 127.1, 71.0, 68.7, 43.6, 31.5 ppm; ν_{max}(KBr)/cm^{-1} 3054, 2926, 1644, 1500, 1446, 1138; MS (EI) m/z 139, 175, 209, 245, 280, 310; HRMS(ESI): m/z calcd for $C_{12}H_{10}Cl_4NaO$ $[M + Na]^+$ 332.9378, found 332.9378.



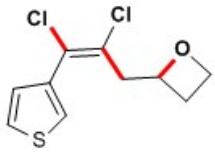
(Z)-2-(2,3-dichloro-3-(2,4-dichlorophenyl)allyl)oxetane (5k)

Yield: 68% (31.6 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (s, 1H), 7.32 (d, J = 8.4 Hz, 1H), 7.25-7.17 (m, 1H), 3.95-3.84 (m, 1H), 3.80-3.66 (m, 3H), 3.17-2.89 (m, 1H), 2.19-1.97 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.8, 136.5, 136.2, 134.3, 131.6, 131.5, 130.1, 127.8, 70.5, 68.4, 43.8, 31.0 ppm; ν_{max}(KBr)/cm^{-1} 3059, 2926, 1642, 1437, 1405, 1109; MS (EI) m/z 139, 175, 210, 245, 280, 310; HRMS(ESI): m/z calcd for $C_{12}H_{10}Cl_4NaO$ $[M + Na]^+$ 332.9378, found 332.9378.



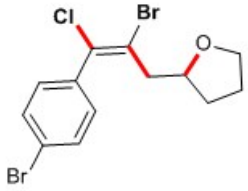
(Z)-2-(2,3-dichloro-3-(naphthalen-1-yl)allyl)oxetane (5l)

Yield: 65% (28.5 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 7.6 Hz, 3H), 7.60-7.54 (m, 2H), 7.48 (d, J = 7.2 Hz, 1H), 7.44 - 7.37 (m, 1H), 3.93-3.82 (m, 1H), 3.77 (d, J = 8.0 Hz, 1H), 3.59 (dd, J = 13.6, 9.2 Hz, 2H), 3.10-3.00 (m, 1H), 2.14 (dq, J = 12.8, 7.6 Hz, 1H), 1.83-1.68 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 135.4, 135.3, 134.2, 133.8, 130.7, 128.6, 127.2, 127.1, 126.6, 125.4, 124.8, 70.7, 68.6, 43.8, 31.1 ppm; ν_{max}(KBr)/cm^{-1} 3049, 2924, 1643, 1564, 1516, 1453, 1405, 1129; MS (EI) m/z 113, 163, 191, 221, 257, 292; HRMS(ESI): m/z calcd for $C_{16}H_{14}Cl_2NaO$ $[M + Na]^+$ 315.0314, found 315.0311.



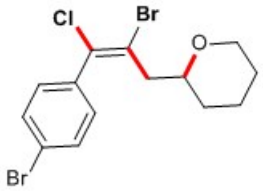
(Z)-2-(2,3-dichloro-3-(thiophen-3-yl)allyl)oxetane (5m)

Yield: 54% (20.1 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35 (d, J = 4.4 Hz, 1H), 7.31 (s, 1H), 7.10 (d, J = 4.0 Hz, 1H), 3.94 (dd, J = 13.6, 8.0 Hz, 1H), 3.86 (t, J = 8.4 Hz, 1H), 3.77 (dd, J = 15.2, 7.2 Hz, 2H), 3.60-3.49 (m, 1H), 2.17 (td, J = 15.2, 7.6 Hz, 1H), 2.06-1.94 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.8, 134.3, 127.9, 126.3, 125.4, 124.6, 71.0, 68.7, 43.6, 31.5 ppm; ν_{max}(KBr)/cm^{-1} 3046, 2928, 1643, 1506, 1455, 1124; MS (EI) m/z 105, 121, 147, 183, 213, 248; HRMS(ESI): m/z calcd for $C_{10}H_{10}Cl_2NaOS$ $[M + Na]^+$ 270.9722, found 270.9724.



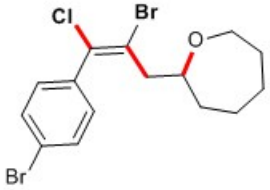
(Z)-2-(2-bromo-3-(4-bromophenyl)-3-chloroallyl)tetrahydrofuran (6a)

Yield: 75% (42.5 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 8.4 Hz, 2H), 4.25 (dq, J = 14.4, 7.2 Hz, 1H), 3.74 (t, J = 6.8 Hz, 2H), 2.71 (dt, J = 17.2, 8.8 Hz, 1H), 2.45 (dd, J = 14.4, 4.4 Hz, 1H), 2.08-1.97 (m, 1H), 1.94-1.81 (m, 1H), 1.80-1.73 (m, 1H), 1.38 (td, J = 15.2, 7.6 Hz, 1H) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.3, 132.1, 131.6, 131.4, 130.8, 129.9, 71.4, 67.9, 43.8, 30.9, 25.6 ppm; ν_{max}(KBr)/cm^{-1} 3046, 2924, 1643, 1515, 1452, 1123; MS (EI) m/z 114, 149, 193, 227, 254, 307, 336, 378; HRMS(ESI): m/z calcd for $C_{13}H_{13}Br_2ClNaO$ $[M + Na]^+$ 400.8914, found 400.8911.



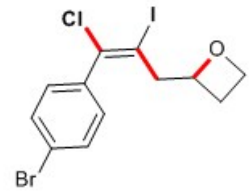
(Z)-2-(2-bromo-3-(4-bromophenyl)-3-chloroallyl)tetrahydro-2H-pyran (6b)

Yield: 61% (35.8 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, J = 8.4 Hz, 2H), 7.22 (d, J = 8.4 Hz, 2H), 3.79 (dd, J = 14.4, 7.2 Hz, 1H), 3.74-3.59 (m, 2H), 2.59 (dt, J = 15.2, 7.6 Hz, 1H), 2.54-2.43 (m, 1H), 1.94-1.84 (m, 2H), 1.79 (dd, J = 14.0, 7.2 Hz, 2H), 1.45-1.33 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.2, 131.8, 130.3, 130.0, 127.8, 123.2, 77.8, 67.6, 35.3, 34.9, 31.2, 25.6 ppm; ν_{max}(KBr)/cm^{-1} 3060, 2926, 1645, 1505, 1416, 1114; MS (EI) m/z 114, 128, 150, 229, 281, 316, 357, 392; HRMS(ESI): m/z calcd for $C_{14}H_{15}Br_2ClNaO$ $[M + Na]^+$ 414.9070, found 414.9064



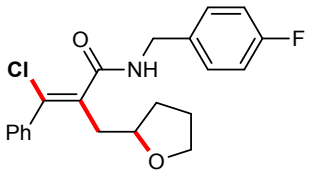
(Z)-2-(2-bromo-3-(4-bromophenyl)-3-chloroallyl)oxepane (6c)

Yield: 48% (29.2 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, J = 8.4 Hz, 2H), 7.20 (d, J = 8.4 Hz, 2H), 3.82 (dd, J = 14.4, 7.2 Hz, 1H), 3.67 (dd, J = 13.6, 7.2 Hz, 2H), 2.45 (t, J = 7.2 Hz, 2H), 1.92-1.80 (m, 2H), 1.73-1.53 (m, 4H), 1.42-1.34 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 131.8, 130.3, 129.9, 128.1, 123.1, 78.8, 67.7, 37.9, 34.3, 31.3, 25.7, 25.6 ppm; ν_{max}(KBr)/cm^{-1} 3056, 2928, 1646, 1456, 1423, 1125; MS (EI) m/z 105, 128, 162, 195, 207, 242, 291, 327, 371, 406; HRMS(ESI): m/z calcd for $C_{15}H_{17}Br_2ClNaO$ $[M + Na]^+$ 428.9227, found 428.9225.



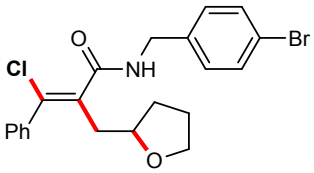
(Z)-2-(3-(4-bromophenyl)-3-chloro-2-iodoallyl)oxetane (8)

Yield: 77% (47.6 mg) as a yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, J = 8.4 Hz, 2H), 7.18 (d, J = 8.4 Hz, 2H), 3.94 (dd, J = 13.2, 8.4 Hz, 1H), 3.81-3.68 (m, 3H), 3.21 (p, J = 8.0 Hz, 1H), 2.13 (dq, J = 15.6, 7.6 Hz, 1H), 2.02-1.84 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 132.1, 131.2, 130.2, 129.2, 123.5, 71.9, 68.6, 44.8, 32.6 ppm; ν_{max}(KBr)/cm^{-1} 3026, 2930, 1645, 1486, 1453, 1108; MS (EI) m/z 115, 141, 176, 220, 267, 347, 382, 412; HRMS(ESI): m/z calcd for $C_{12}H_{11}BrClINaO$ $[M + Na]^+$ 434.8619, found 434.8616.



(Z)-3-Chloro-*N*-(4-fluorobenzyl)-3-phenyl-2-((tetrahydrofuran-2-yl)methyl)acrylamide (10a)

Yield: 78% (58.2 mg) as a white solid; mp = 133.4 - 135.0 ^{o}C;^{1} H NMR (400 MHz, $CDCl_3$) δ 7.42 - 7.34 (m, 7H), 7.03 (t, J = 8.6 Hz, 2H), 6.74 - 6.65 (m, 1H), 4.61 (dd, J = 14.8, 6.0 Hz, 1H), 4.51 (dd, J = 14.8, 5.6 Hz, 1H), 3.93 - 3.84 (m, 1H), 3.70 (dd, J = 14.8, 6.8 Hz, 1H), 3.61 (dd, J = 15.0, 7.2 Hz, 1H), 2.57 (dd, J = 14.2, 3.6 Hz, 1H), 2.37 (dd, J = 14.2, 10.0 Hz, 1H), 1.96-1.85 (m, 1H), 1.77 (dt, J = 14.4, 6.8 Hz, 2H), 1.34 (ddd, J = 14.8, 12.0, 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 162.2 (d, J = 245.6 Hz), 137.3, 134.3, 133.8 (d, J = 3.1 Hz), 130.5, 129.7, 129.6, 128.9 (d, J = 3.2 Hz), 128.4, 115.5 (d, J = 21.4 Hz), 76.9, 67.7, 42.9, 37.9, 31.4, 25.5 ppm; ν_{max}(KBr)/cm^{-1} 3362, 3028, 2936, 1644, 1456, 1408, 756; MS (EI) m/z 71, 109, 207, 268, 303, 373; HRMS(ESI): m/z calcd for $C_{21}H_{21}ClFNNaO_2$ $[M + Na]^+$ 396.1137, found 396.1143.



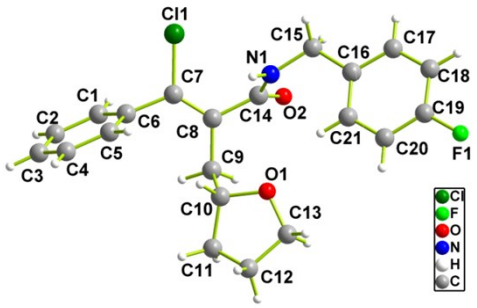
(Z)-*N*-(4-Bromobenzyl)-3-chloro-3-phenyl-2-((tetrahydrofuran-2-yl)methyl)acrylamide (10b)

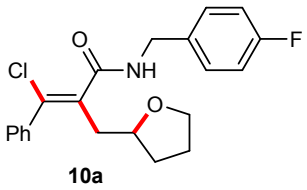
Yield: 71% (46.1 mg) as a white solid; mp = 125.2 - 126.8 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 - 7.47 (m, 2H), 7.45 - 7.36 (m, 5H), 7.29 (d, J = 7.2 Hz, 2H), 6.82 - 6.71 (m, 1H), 4.61 (dd, J = 15.0, 6.0 Hz, 1H), 4.52 (dd, J = 15.0, 5.8 Hz, 1H), 3.95 - 3.87 (m, 1H), 3.77 - 3.70 (m, 1H), 3.68 - 3.61 (m, 1H), 2.58 (dd, J = 14.2, 3.6 Hz, 1H), 2.39 (dd, J = 14.2, 10.0 Hz, 1H), 1.96-1.87 (m, 1H), 1.83 - 1.77 (m, 1H), 1.41 - 1.33 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 137.3, 137.1,

134.2, 131.7, 130.6, 129.7, 128.9, 128.9, 128.4, 121.3, 77.3, 67.8, 43.0, 37.9, 31.4, 25.5 ppm; ν_{max}(KBr)/cm^{-1} 3356, 3030, 2938, 1642, 1476, 1413, 768; MS (EI) m/z 71, 115, 169, 264, 328, 365, 433; HRMS(ESI): m/z calcd for $C_{21}H_{21}BrClNNaO_2$ $[M + Na]^+$ 456.0336, found 456.0340.

X-ray Crystallographic Analysis for Product 10a

The CCDC number of compound **10a** is 1491284.



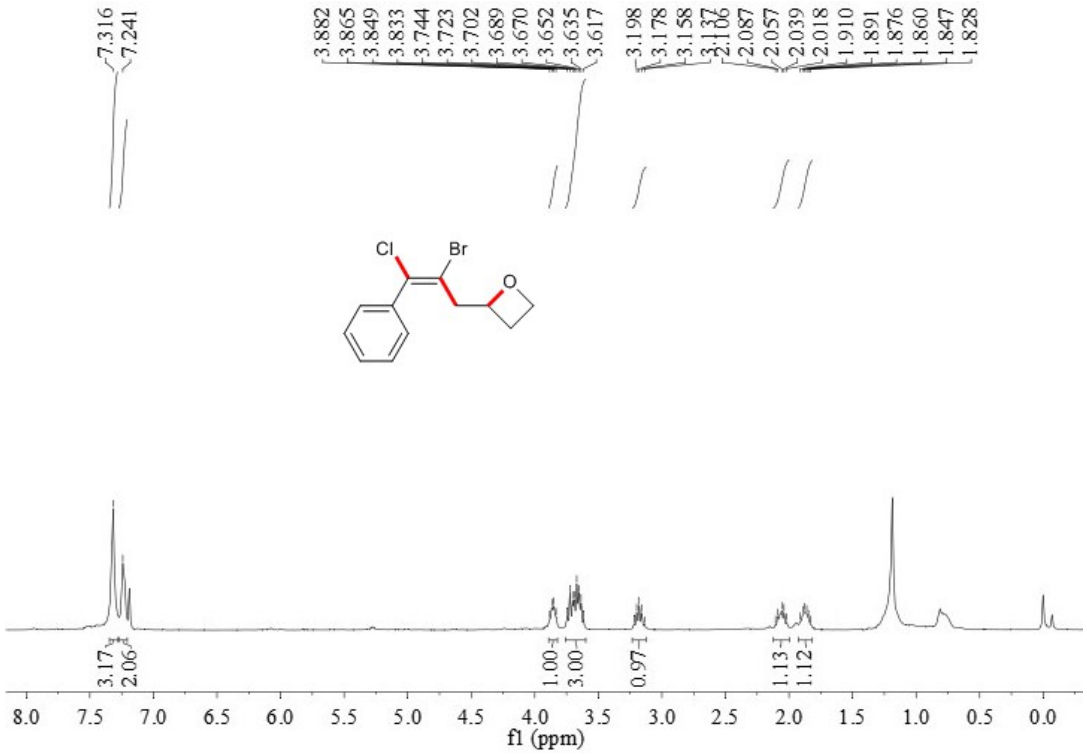


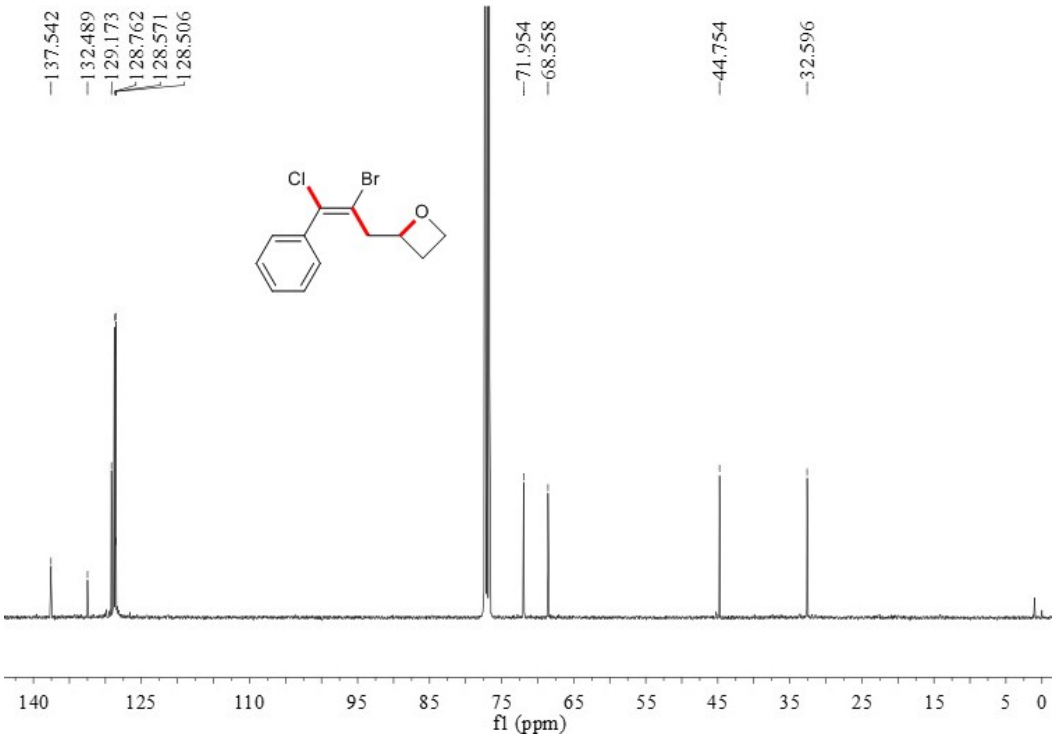
10a

Crystal Data and Structure Refinement for Product **10a**

Empirical formula	$C_{21}H_{21}ClFNO_2$
Formula weight	373.84
Temperature	150(10) K
Wavelength	1.54184 Å
Crystal system	monoclinic
Space group	P 1 21/c 1
Unit cell dimensions	a= 9.4639(2) Å, α= 90.00°
	b= 21.8249(5) Å, β= 104.752(3)°
	c= 9.3192(2) Å, γ= 90.00°
Density (calculated)	1.334
Absorption coefficient	2.024
F(000)	784
Crystal size	0.2×0.1×0.1
Theta range for data collection	4.05 to 74.11
Index ranges	-10<=h<=11, -26<=k<=24, -11<=l<=9
Reflections collected	12068
Independent reflections	3691
Completeness to theta = 25.00°	99.94%
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3691/0/235
Goodness-of-fit on F^2	1.033
Final R indices [I>2sigma(I)]	R1 = 0.0446, wR2 = 0.1182
R indices (all data)	R1 = 0.0476, wR2 = 0.1209

NMR Spectra for all Compounds

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95
85
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65
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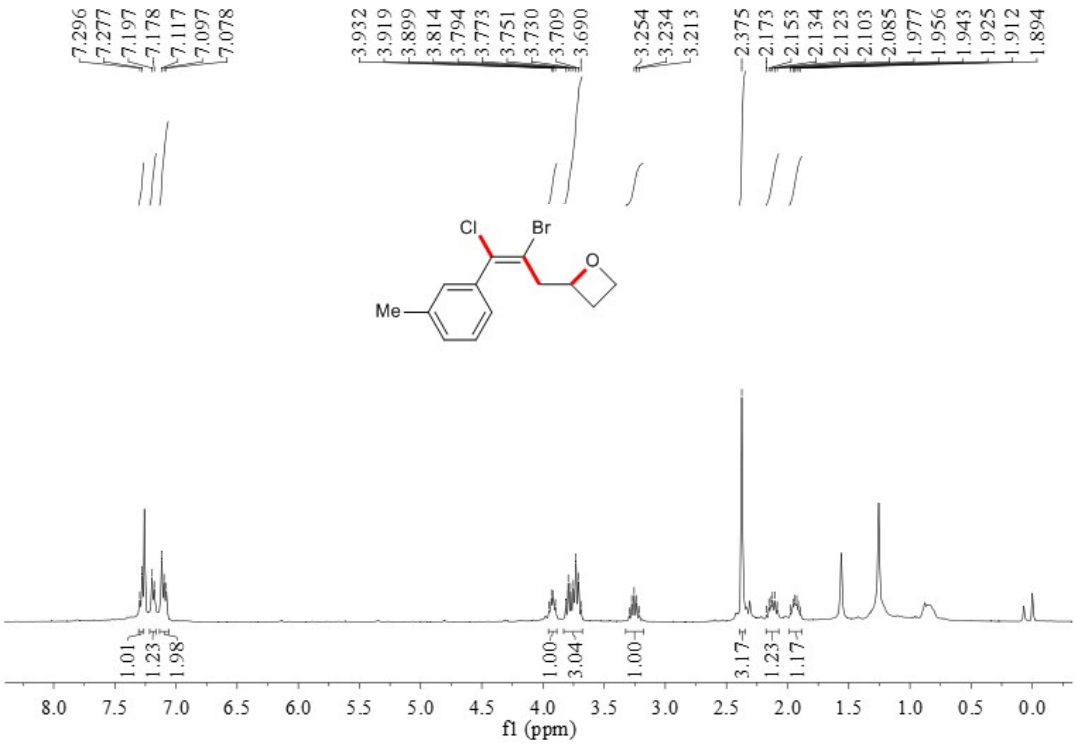
45
35
25
15
5
0
f1 (ppm)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Cl
Br
O
Me
1.01
1.23
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1.00
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1.23
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7.0
6.5
6.0
5.5
5.0
4.5
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3.5
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2.5
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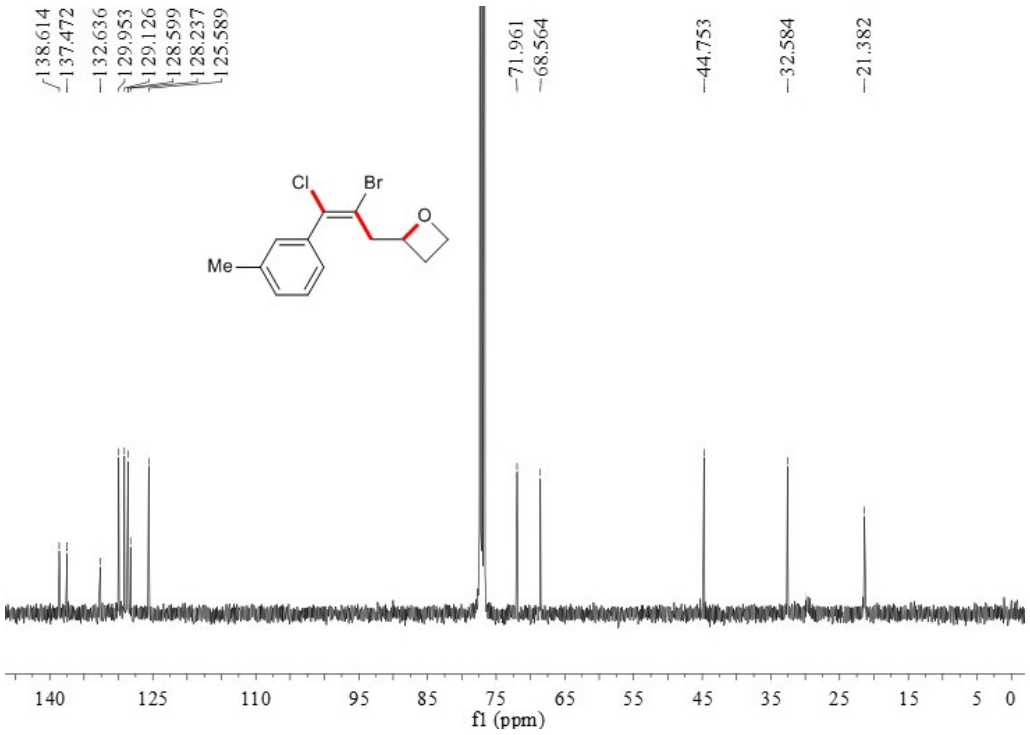
0.0
f1 (ppm)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Cl
Br
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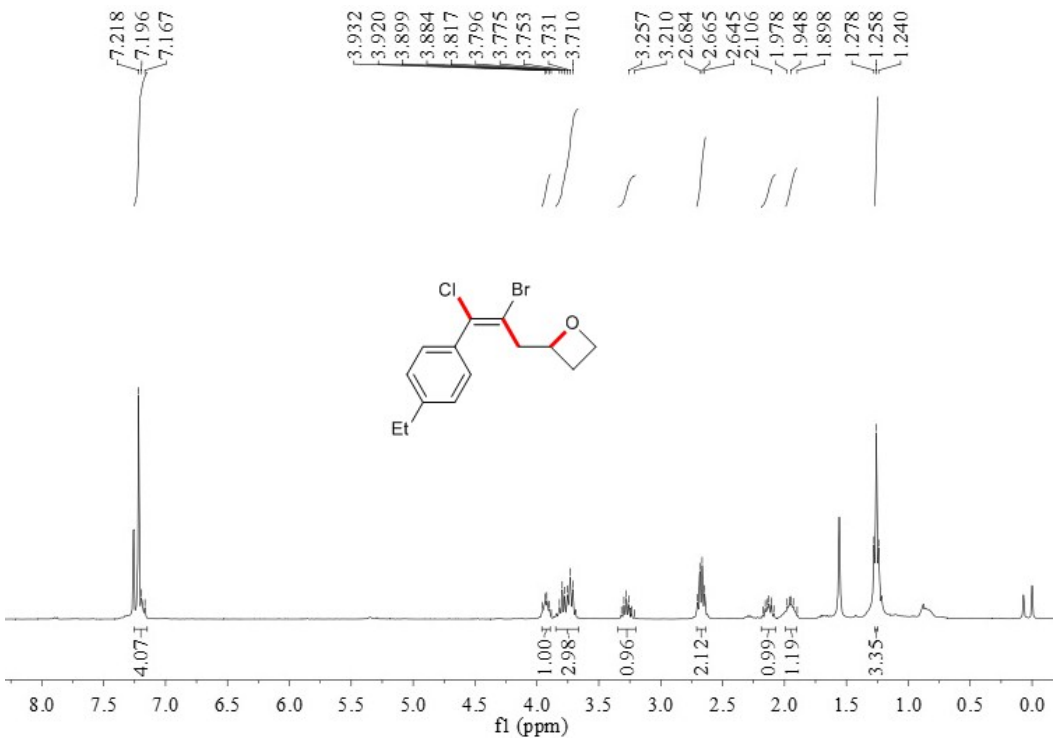
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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7.167
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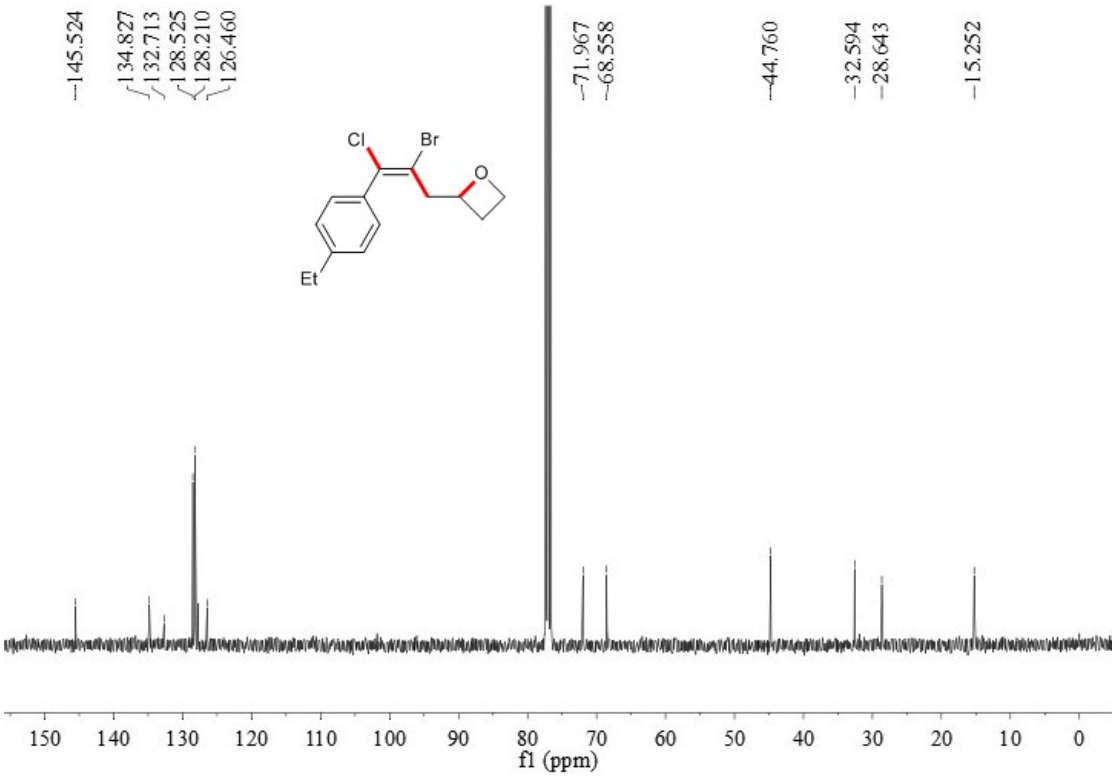
3.817
3.796
3.775
3.753
3.731
3.710
3.257
3.210
2.684
2.665
2.645
2.106
1.978
1.948
1.898
1.278
1.258
1.240
Cl
Br
O
Et
4.07
1.00
2.98
0.96
2.12
0.99
1.19
3.35
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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134.827
132.713
128.525
128.210
126.460
71.967
68.558
44.760
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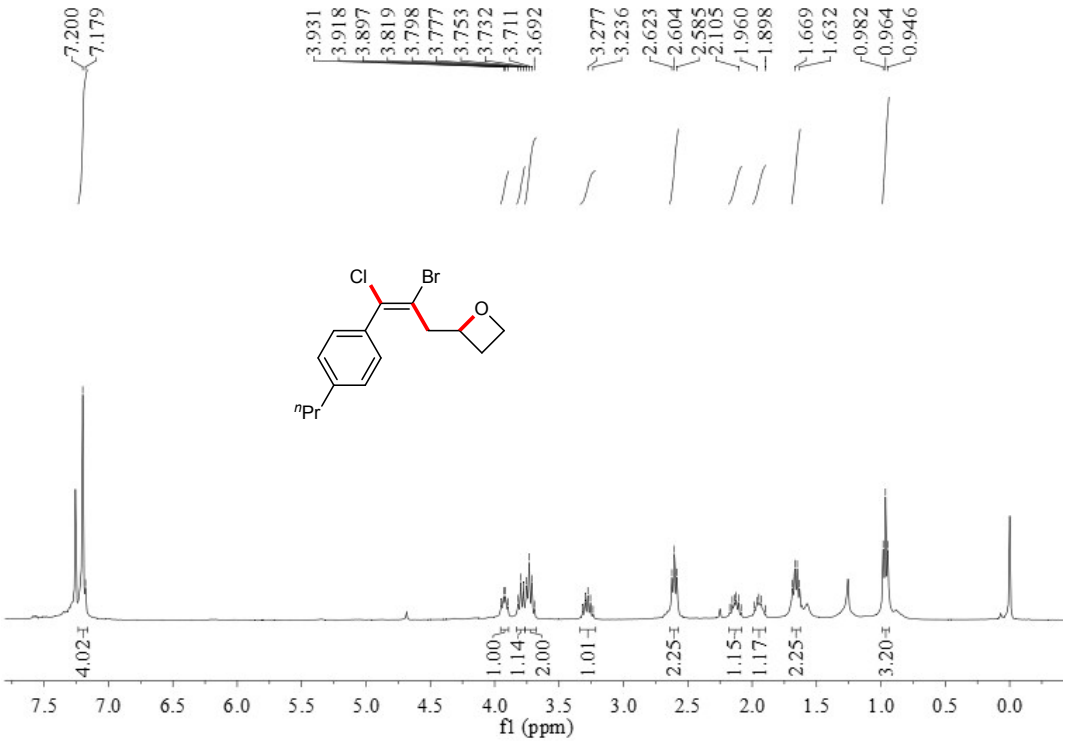
28.643
15.252
Cl
Br
O
Et
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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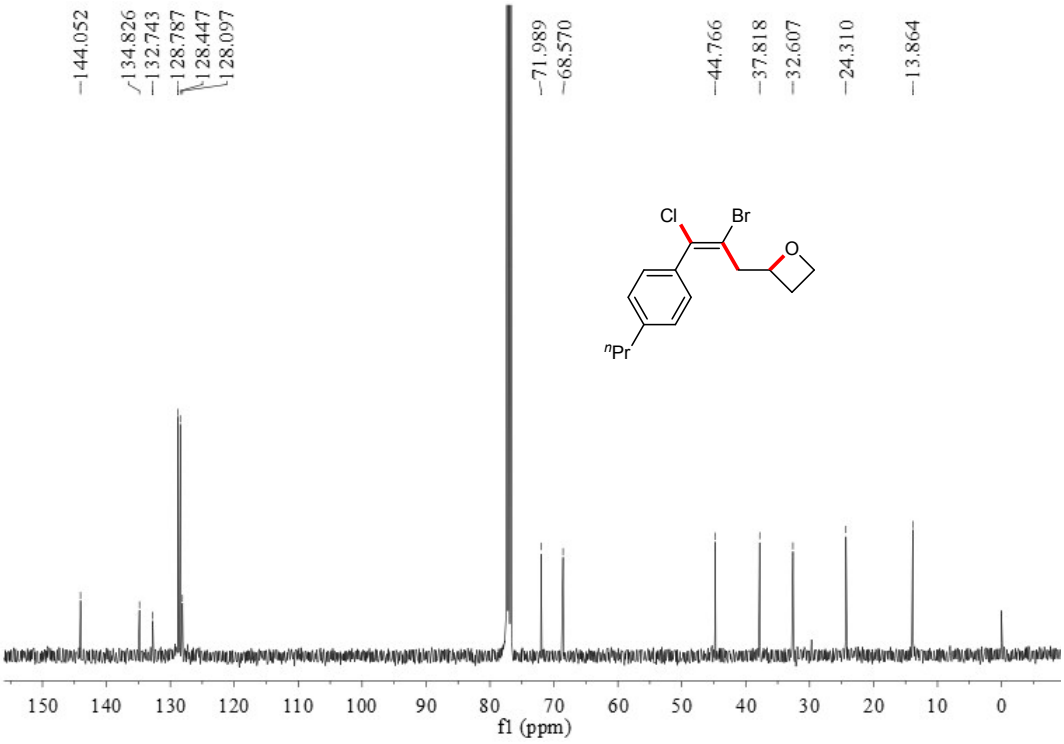
7.179
3.931
3.918
3.897
3.819
3.798
3.777
3.753
3.732
3.711
3.692
3.277
3.236
2.623
2.604
2.585
2.105
1.960
1.898
1.669
1.632
0.982
0.964
0.946
Cl
Br
O
nPr
4.02
1.00
1.14
2.00
1.01
2.25
1.15
1.17
2.25
3.20
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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132.743
128.787
128.447
128.097
71.989
68.570
44.766
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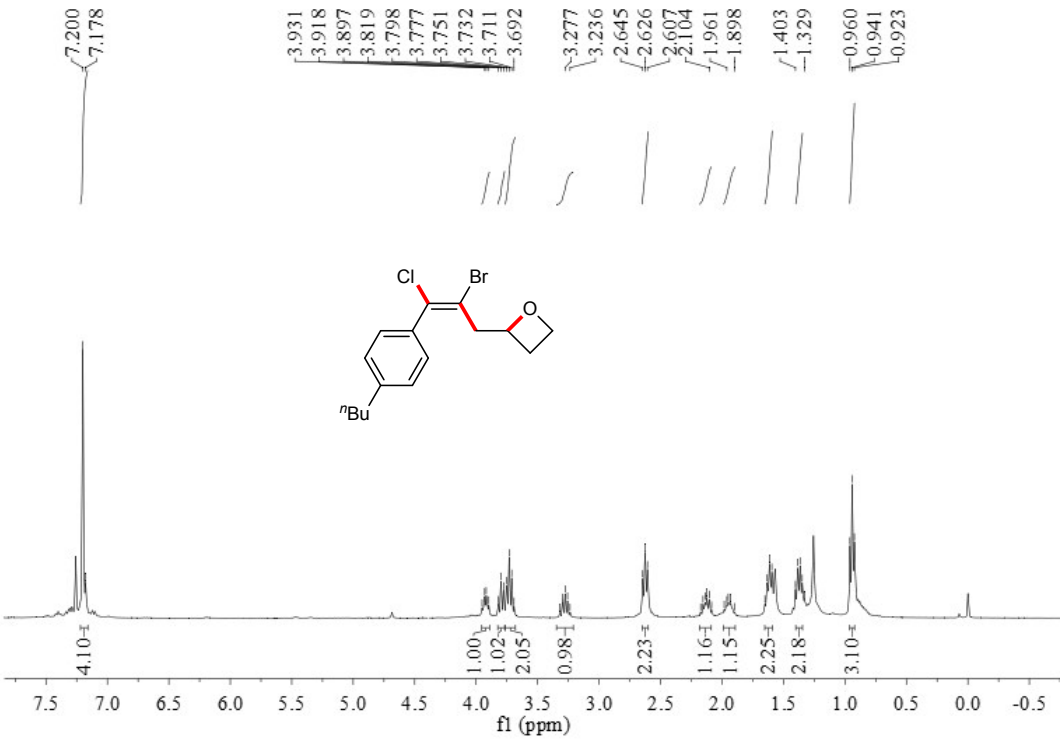
24.310
13.864
Cl
Br
O
nPr
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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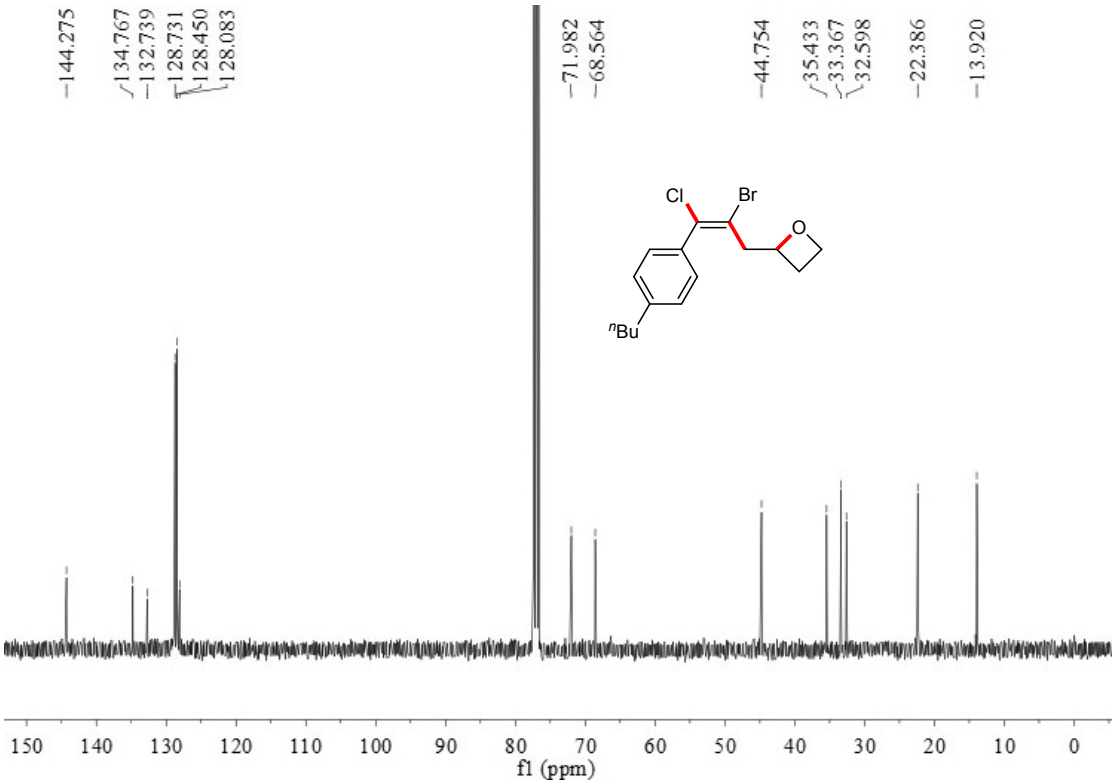
7.178
3.931
3.918
3.897
3.819
3.798
3.777
3.751
3.732
3.711
3.692
3.277
3.236
2.645
2.626
2.607
2.104
1.961
1.898
1.403
1.329
0.960
0.941
0.923
Cl
Br
O
nBu
4.10
1.00
1.02
2.05
0.98
2.23
1.16
1.15
2.25
2.18
3.10
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.731
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68.564
44.754
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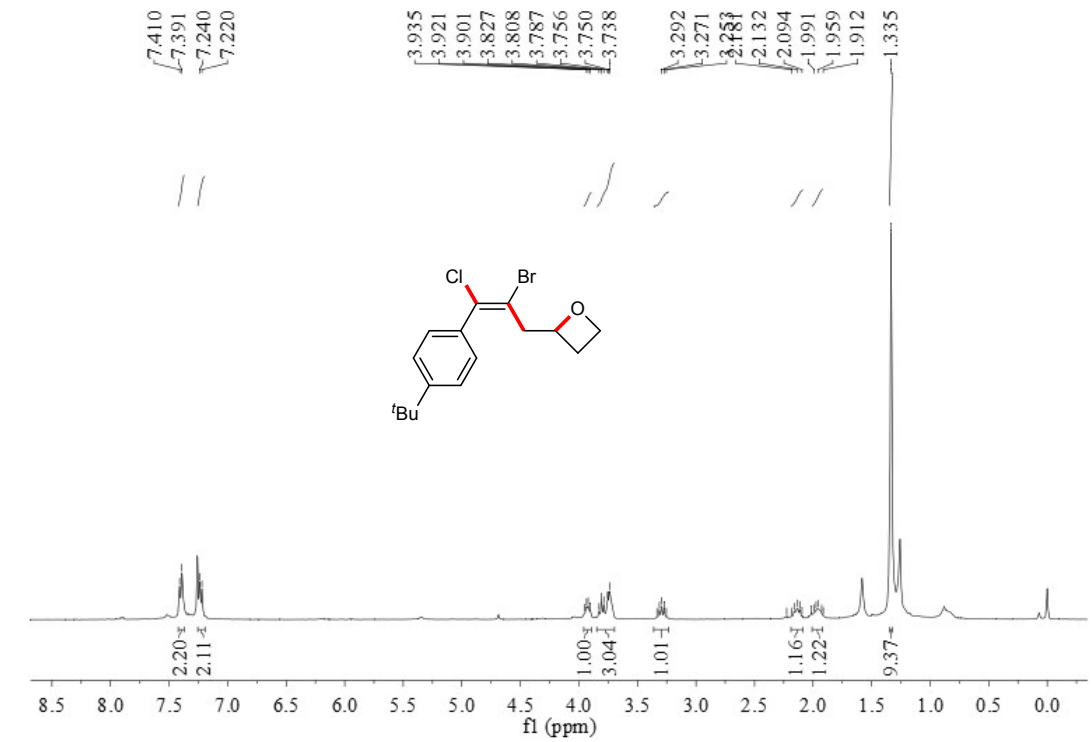
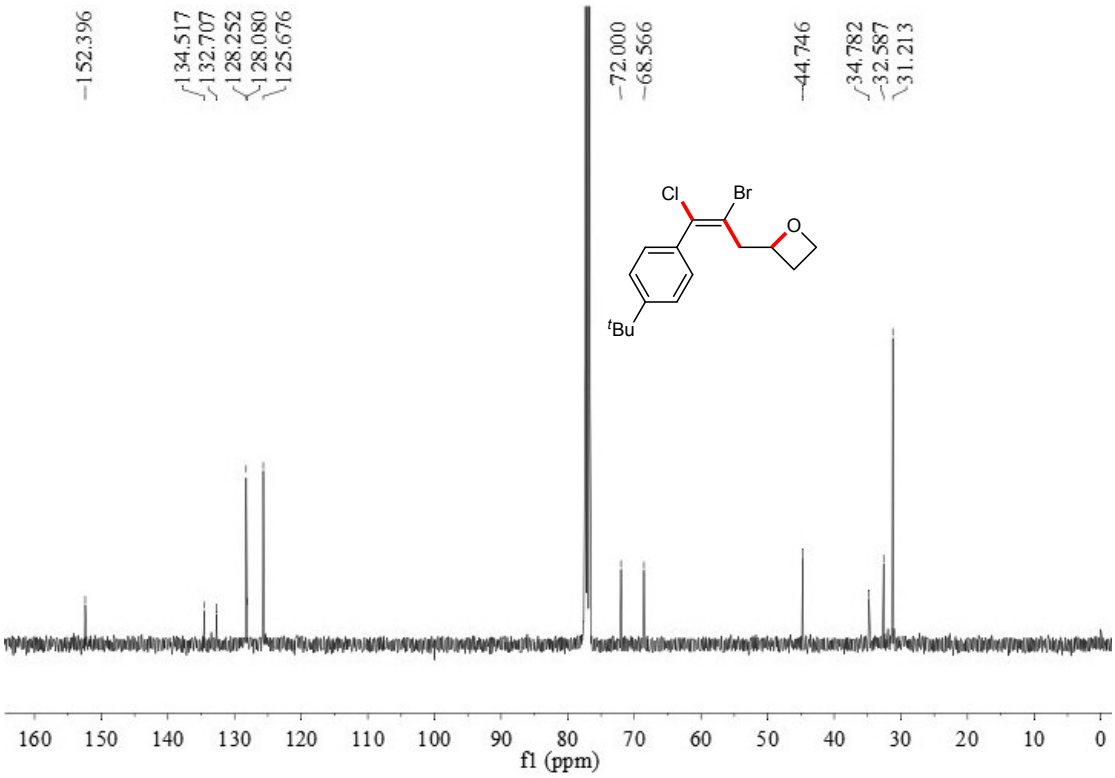
22.386
13.920
Cl
Br
O
nBu
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.410
7.391
7.240
7.220
3.935
3.921
3.901
3.827
3.808
3.787
3.756
3.750
3.738
3.292
3.271
2.132
2.094
1.991
1.959
1.912
1.335
Cl
Br
O
tBu
2.20
2.11
1.00
3.04
1.01
1.16
1.22
9.37
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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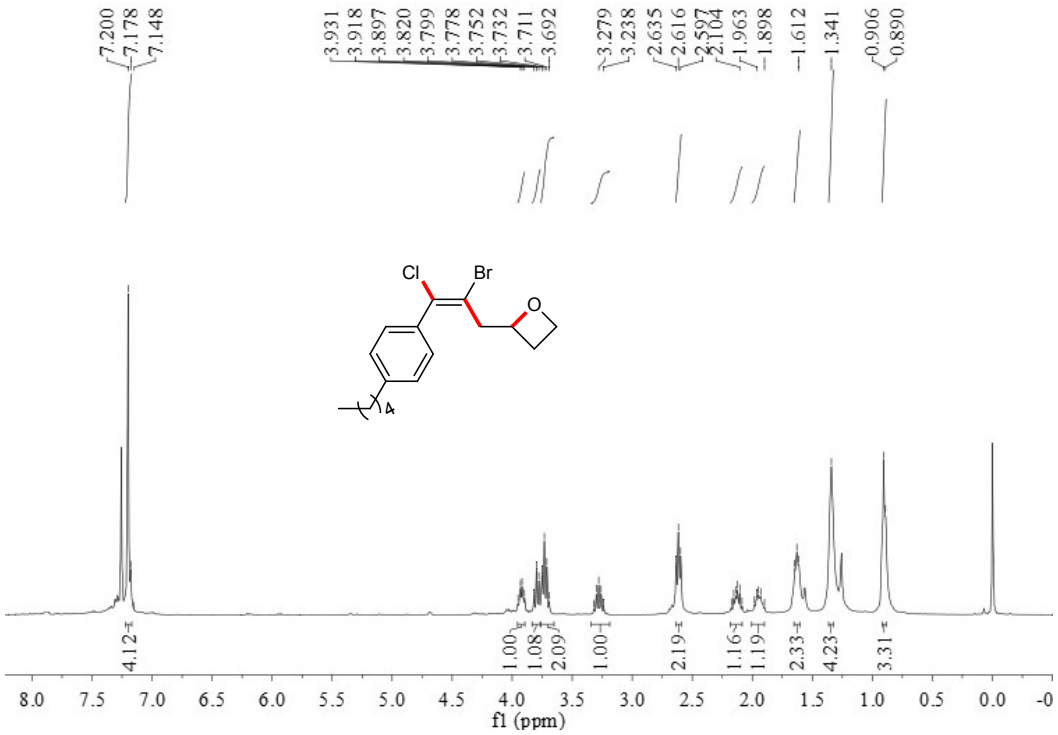
134.517
132.707
128.252
128.080
125.676
72.000
68.566
44.746
34.782
32.587
31.213
Cl
Br
O
tBu
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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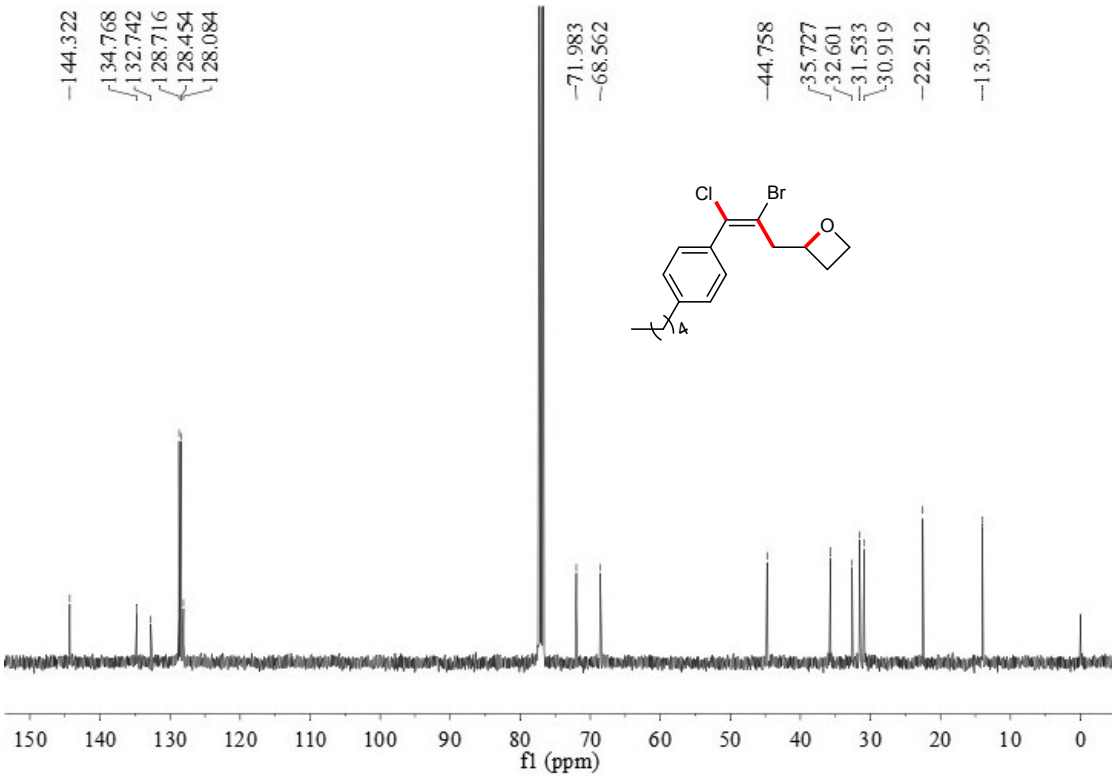
7.178
7.148
3.931
3.918
3.897
3.820
3.799
3.778
3.752
3.732
3.711
3.692
3.279
3.238
2.635
2.616
2.597
2.104
1.963
1.898
1.612
1.341
0.906
0.890
Cl
Br
O
4.12
1.00
1.08
2.09
1.00
2.19
1.16
1.19
2.33
4.23
3.31
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)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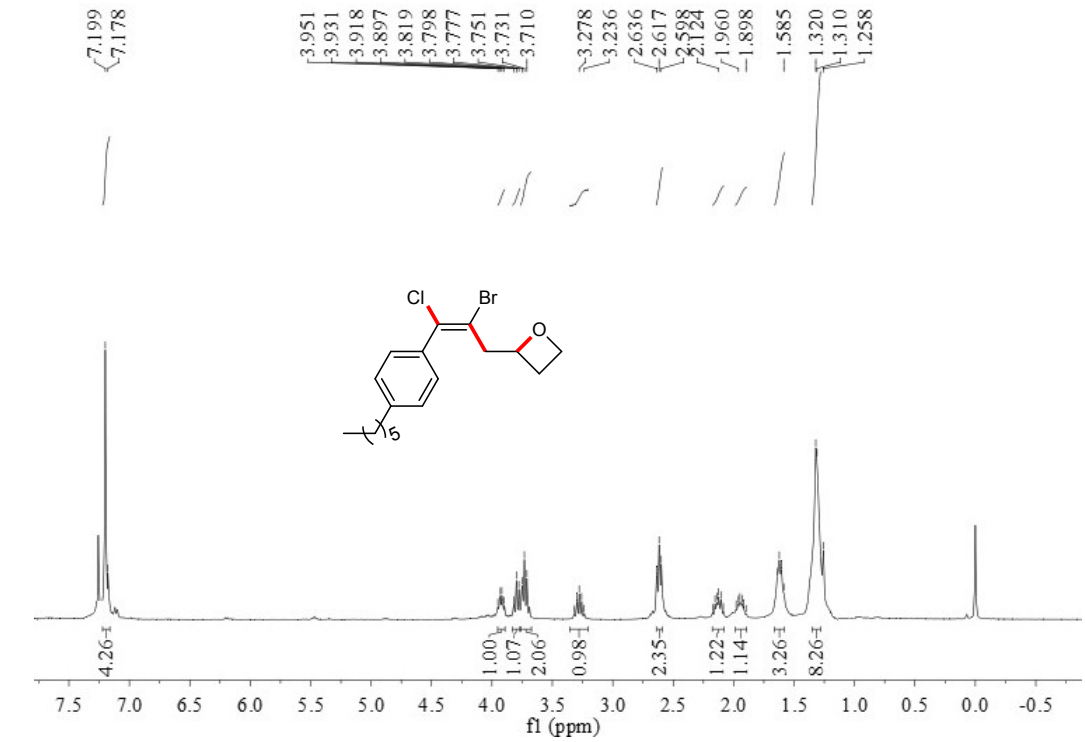
134.768
132.742
128.716
128.454
128.084
71.983
68.562
44.758
35.727
32.601
31.533
30.919
22.512
13.995
Cl
Br
O
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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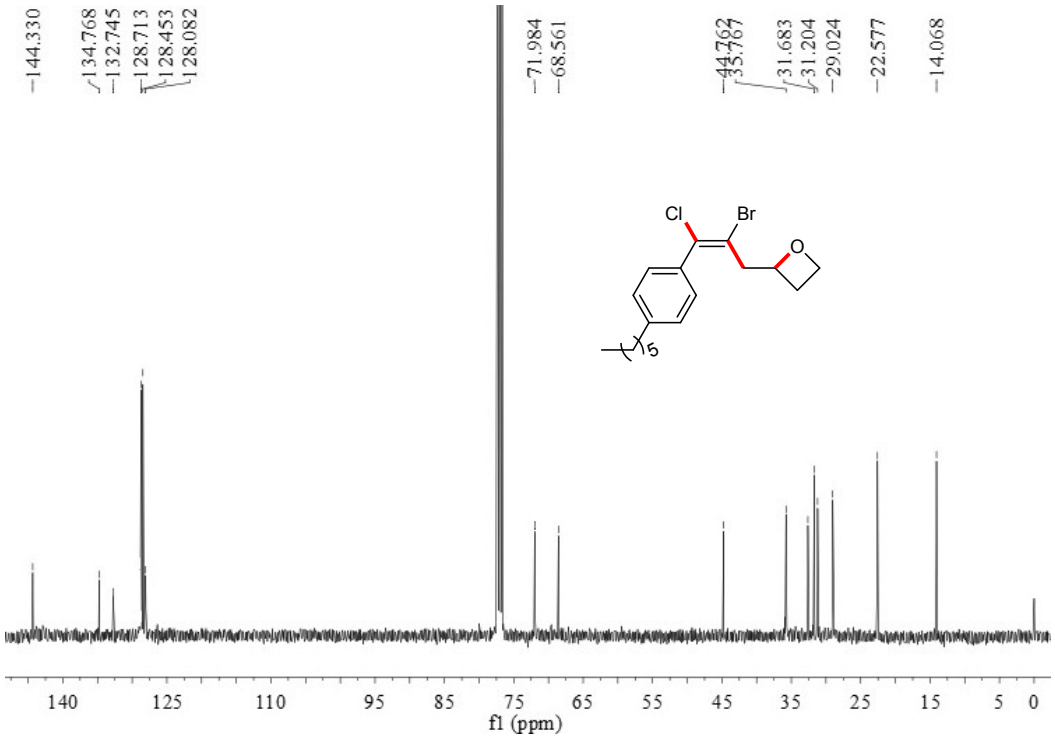
7.178
3.951
3.931
3.918
3.897
3.819
3.798
3.777
3.751
3.731
3.710
3.278
3.236
2.636
2.617
2.598
2.124
1.960
1.898
1.585
1.320
1.310
1.258
Cl
Br
O
4.26
1.00
1.07
2.06
0.98
2.35
1.22
1.14
3.26
8.26
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.082
71.984
68.561
44.762
35.767
31.683
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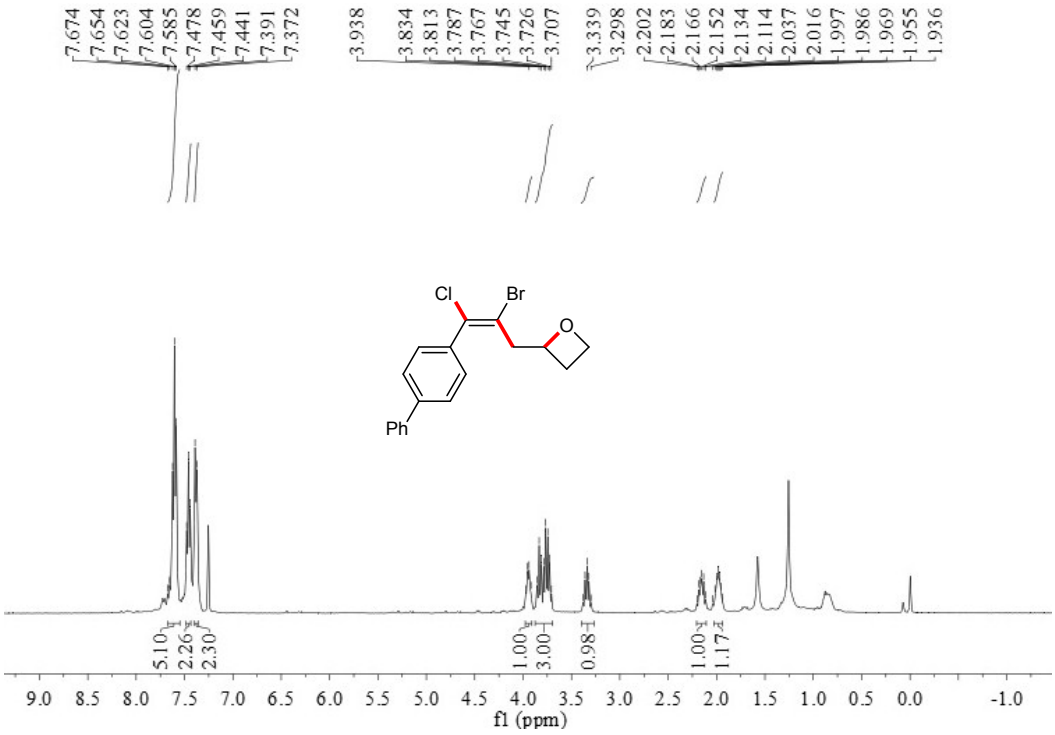
29.024
22.577
14.068
Cl
Br
O
5
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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7.654
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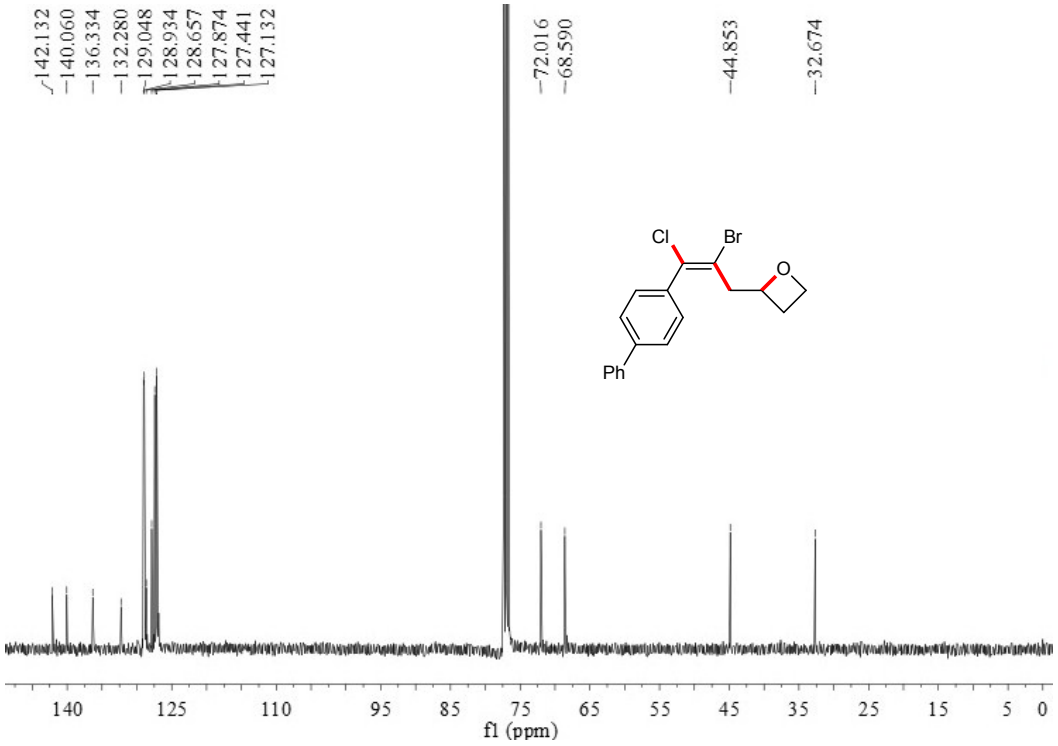
7.604
7.585
7.478
7.459
7.441
7.391
7.372
3.938
3.834
3.813
3.787
3.767
3.745
3.726
3.707
3.339
3.298
2.202
2.183
2.166
2.152
2.134
2.114
2.037
2.016
1.997
1.986
1.969
1.955
1.936
Cl
Br
O
Ph
5.10
2.26
2.30
1.00
3.00
0.98
1.00
1.17
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-1.0
f1 (ppm)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132.280
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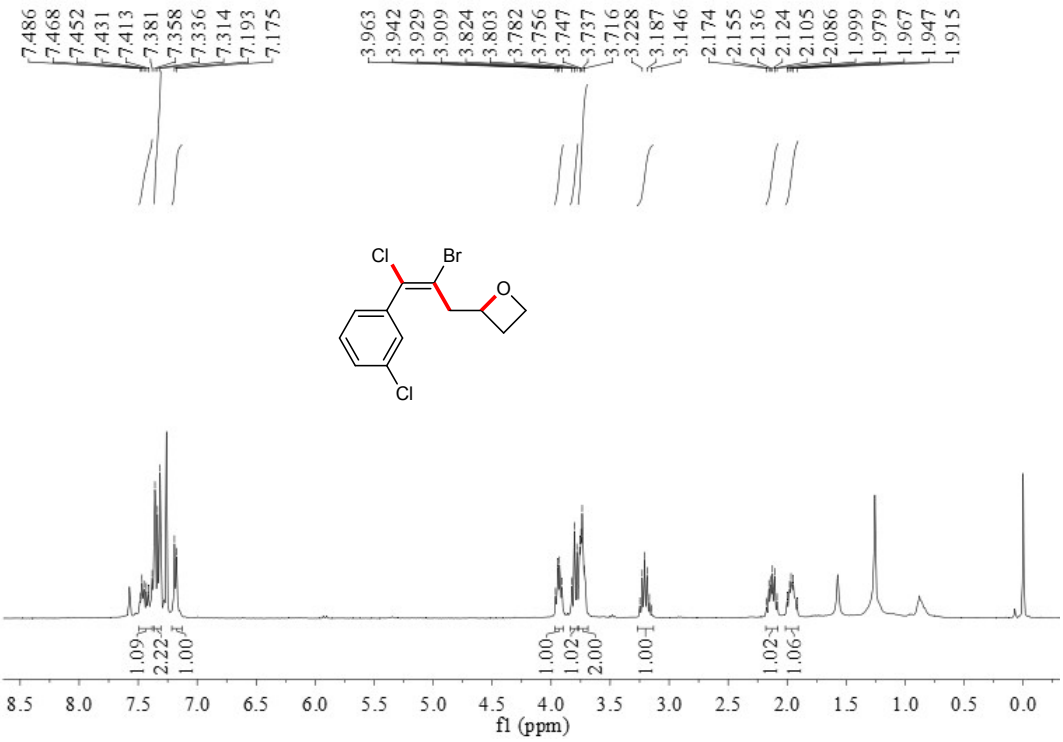
128.934
128.657
127.874
127.441
127.132
72.016
68.590
44.853
32.674
Cl
Br
O
Ph
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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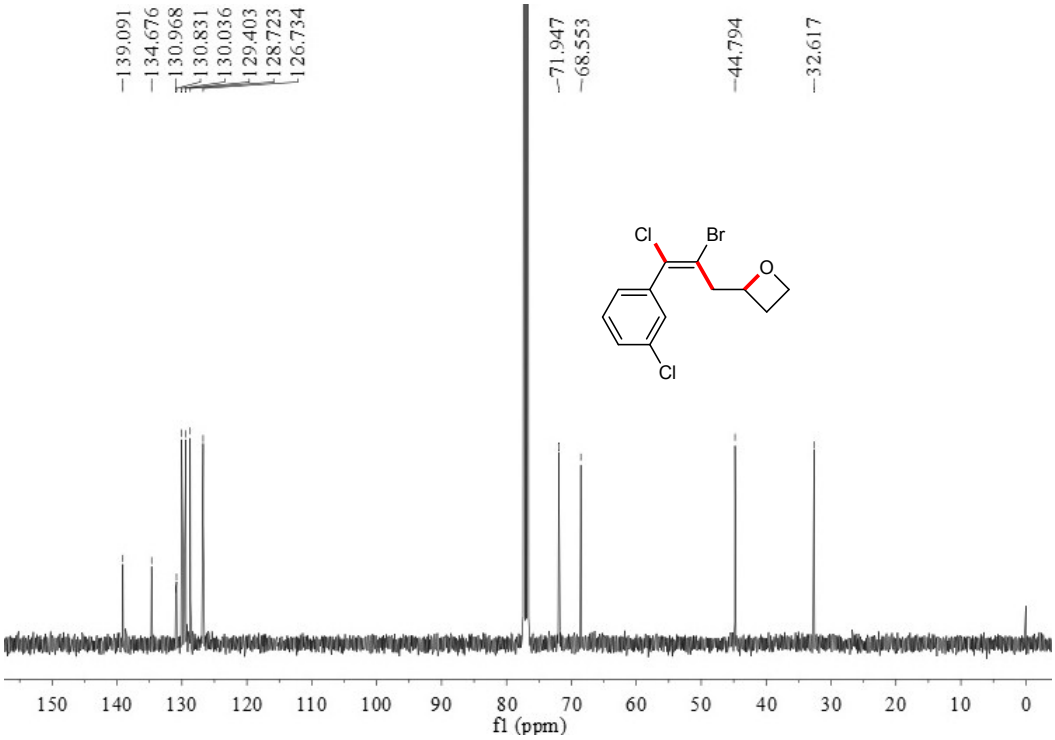
3.942
3.929
3.909
3.824
3.803
3.782
3.756
3.747
3.737
3.716
3.228
3.187
3.146
2.174
2.155
2.136
2.124
2.105
2.086
1.999
1.979
1.967
1.947
1.915
Cl
Br
O
Cl
1.09
2.22
1.00
1.00
1.02
2.00
1.00
1.02
1.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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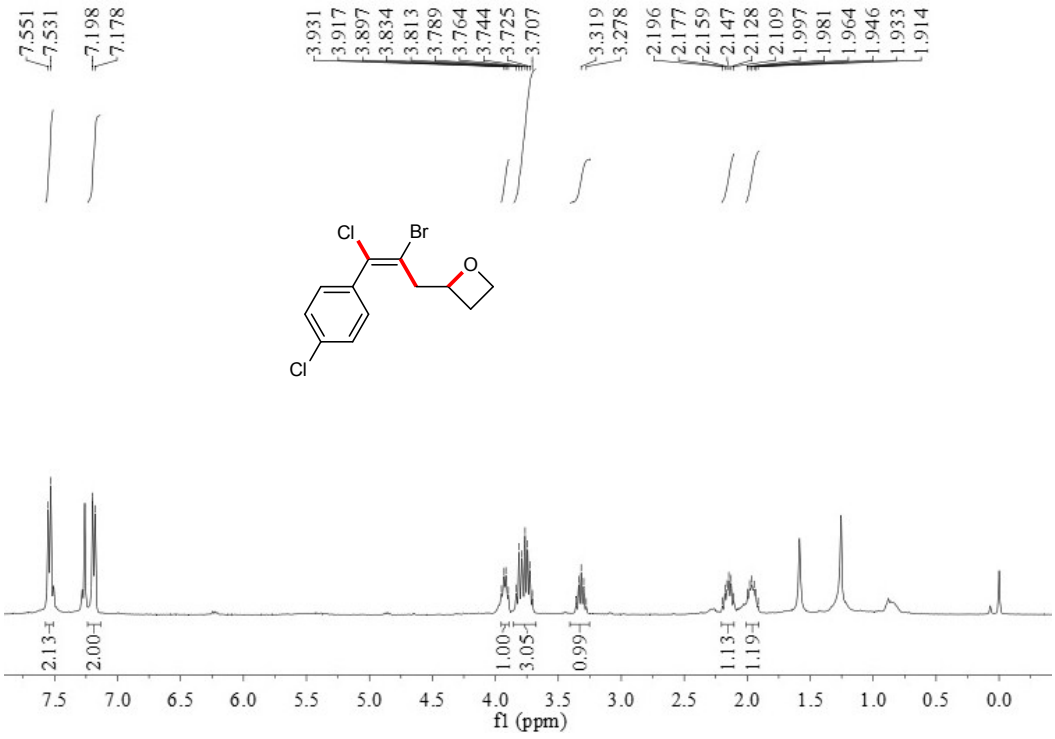
130.036
129.403
128.723
126.734
71.947
68.553
44.794
32.617
Cl
Br
O
Cl
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.178
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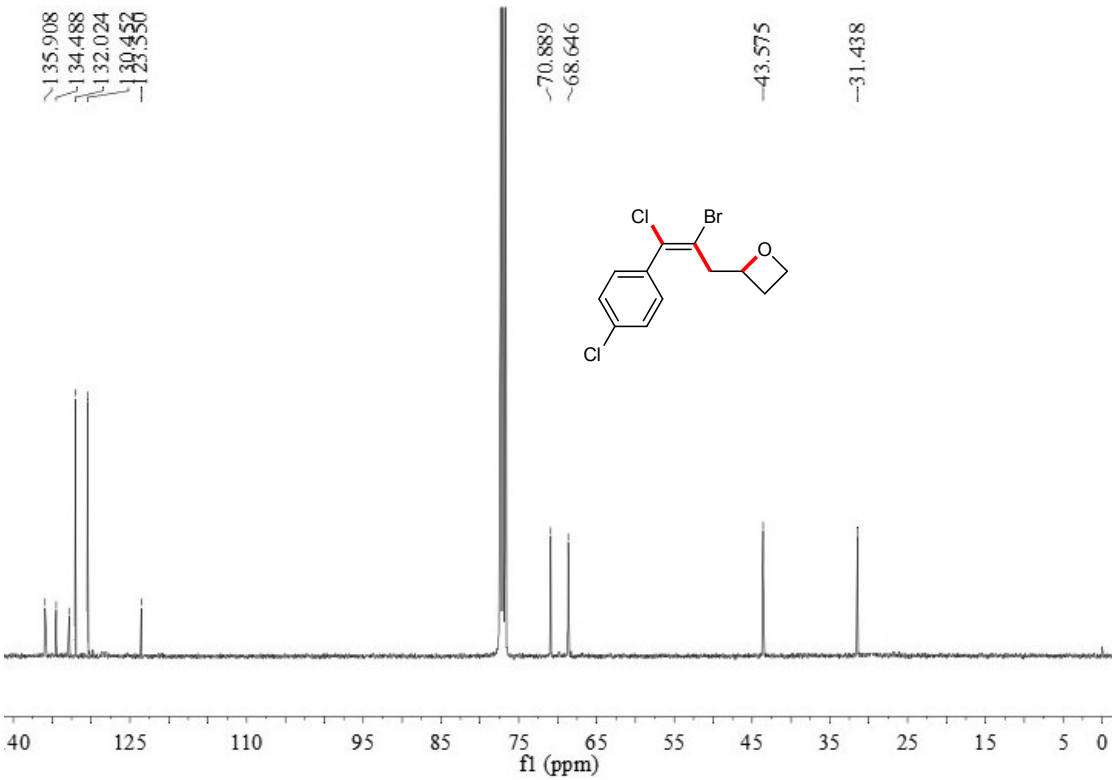
3.917
3.897
3.834
3.813
3.789
3.764
3.744
3.725
3.707
3.319
3.278
2.196
2.177
2.159
2.147
2.128
2.109
1.997
1.981
1.964
1.946
1.933
1.914
Cl
Br
O
Cl
2.13
2.00
1.00
3.05
0.99
1.13
1.19
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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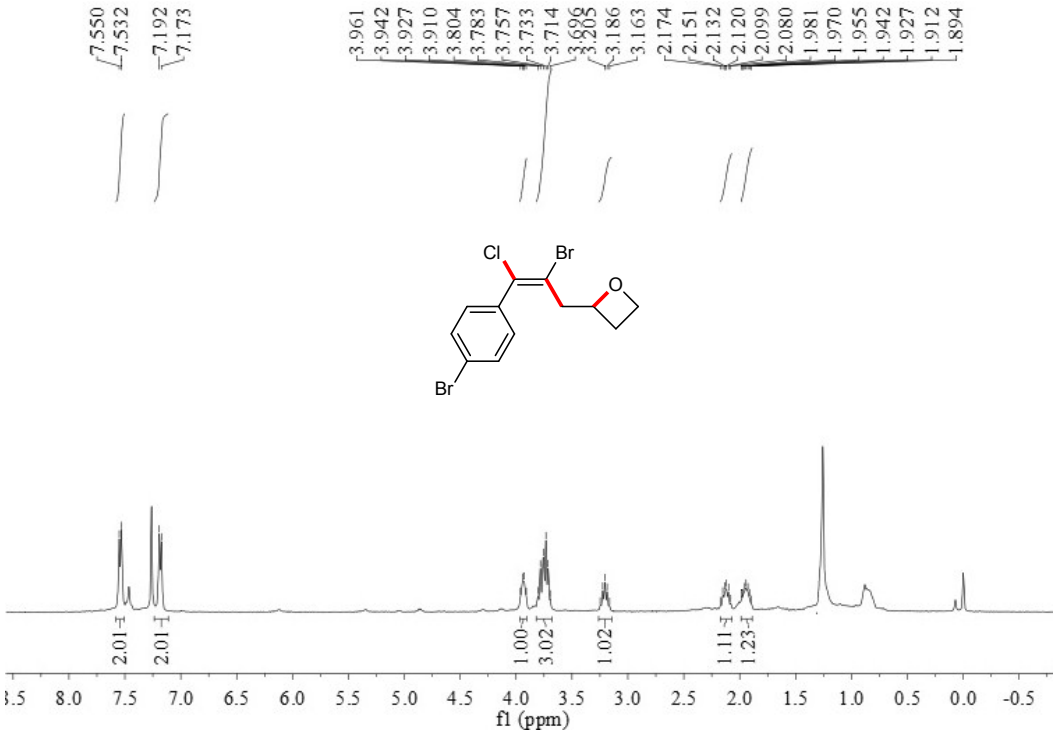
132.024
70.889
68.646
43.575
31.438
Cl
Br
O
Cl
40
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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7.173
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3.942
3.927
3.910
3.804
3.783
3.757
3.733
3.714
3.696
3.205
3.186
3.163
2.174
2.151
2.132
2.120
2.099
2.080
1.981
1.970
1.955
1.942
1.927
1.912
1.894
Cl
Br
O
Br
2.01
2.01
1.00
3.02
1.02
1.11
1.23
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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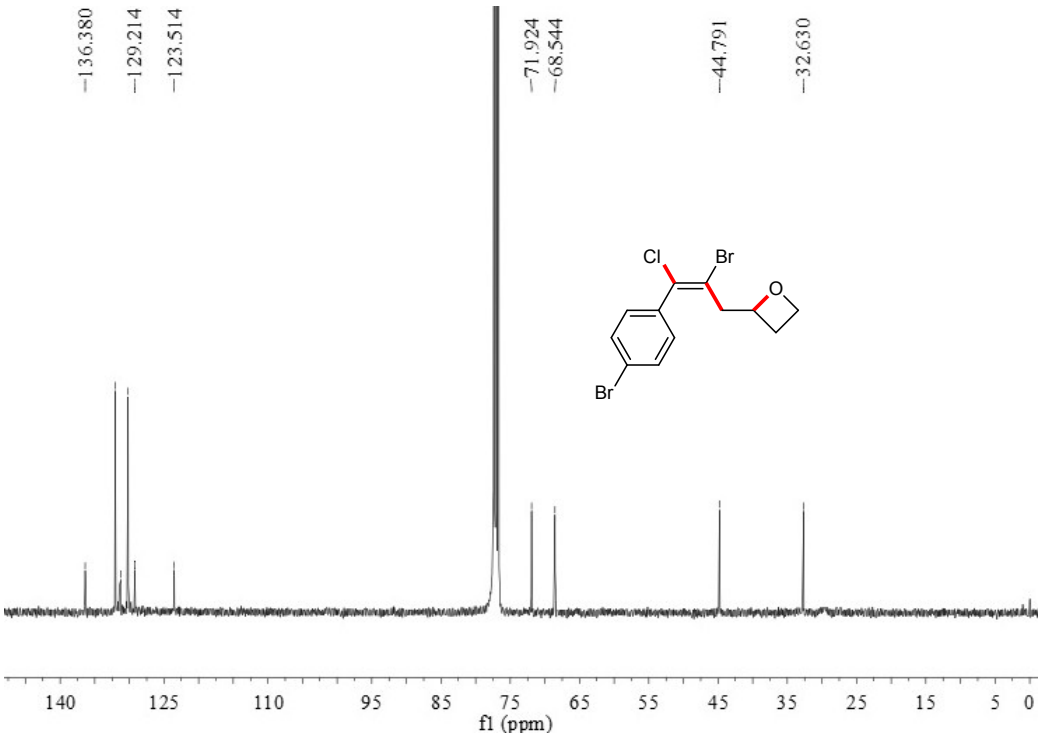
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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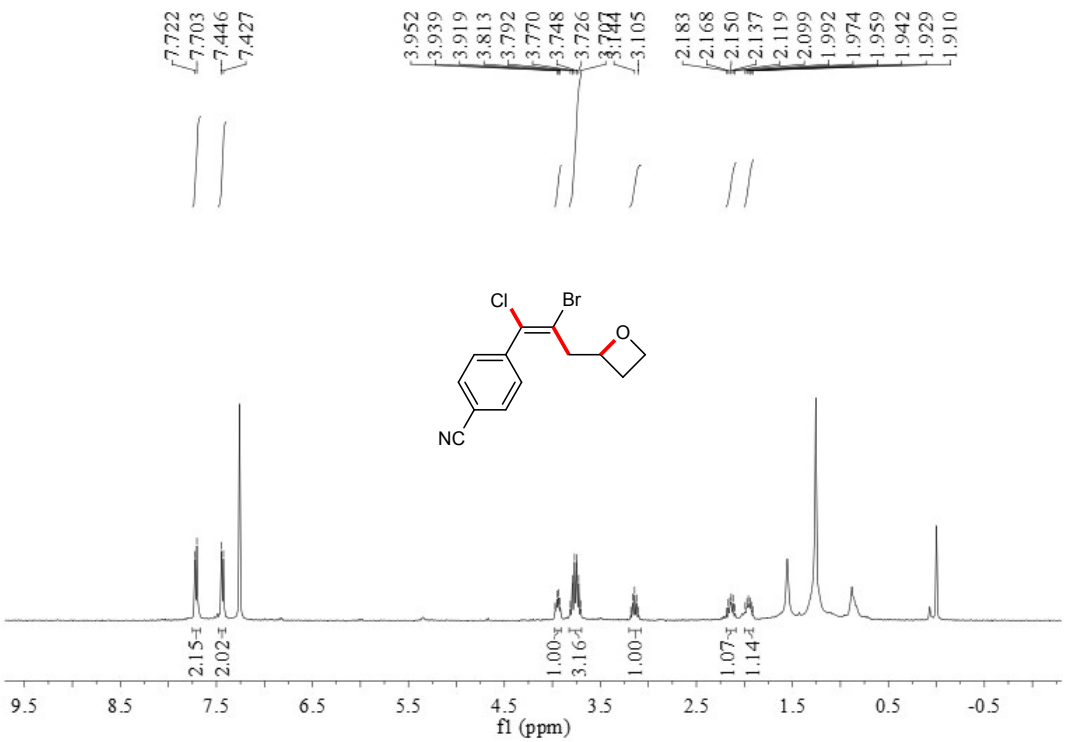
129.214
123.514
71.924
68.544
44.791
32.630
Cl
Br
O
Br
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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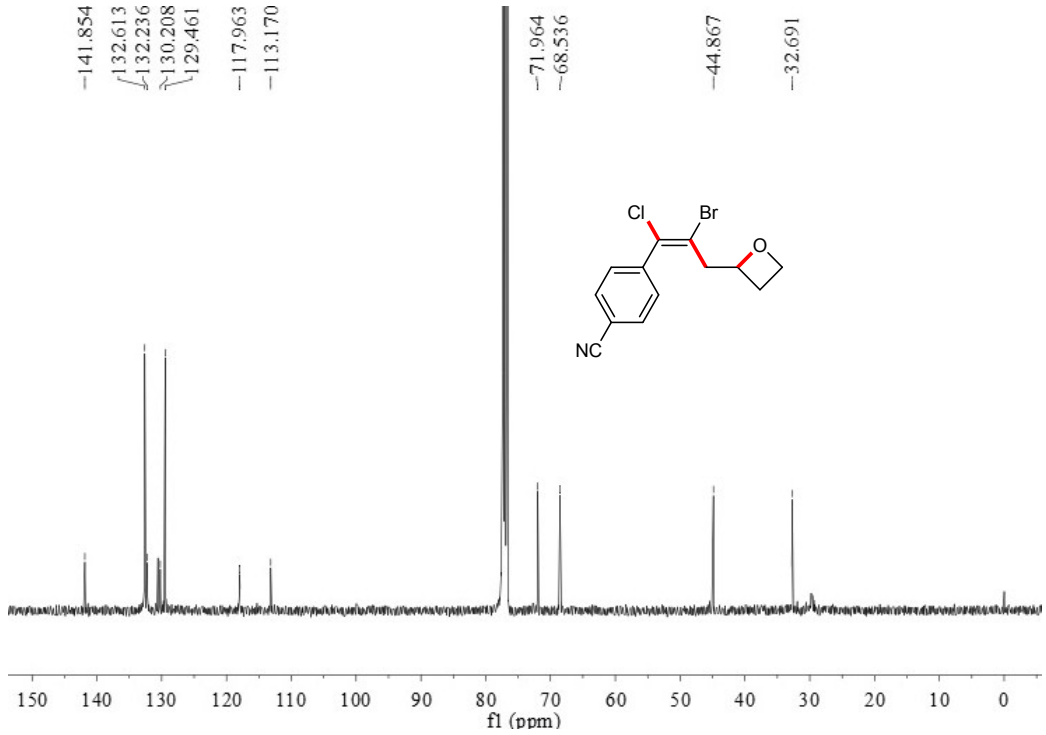
3.707
3.105
2.183
2.168
2.150
2.137
2.119
2.099
1.992
1.974
1.959
1.942
1.929
1.910
Cl
Br
O
NC
2.15
2.02
1.00
3.16
1.00
1.07
1.14
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)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132.236
130.208
129.461
117.963
113.170
71.964
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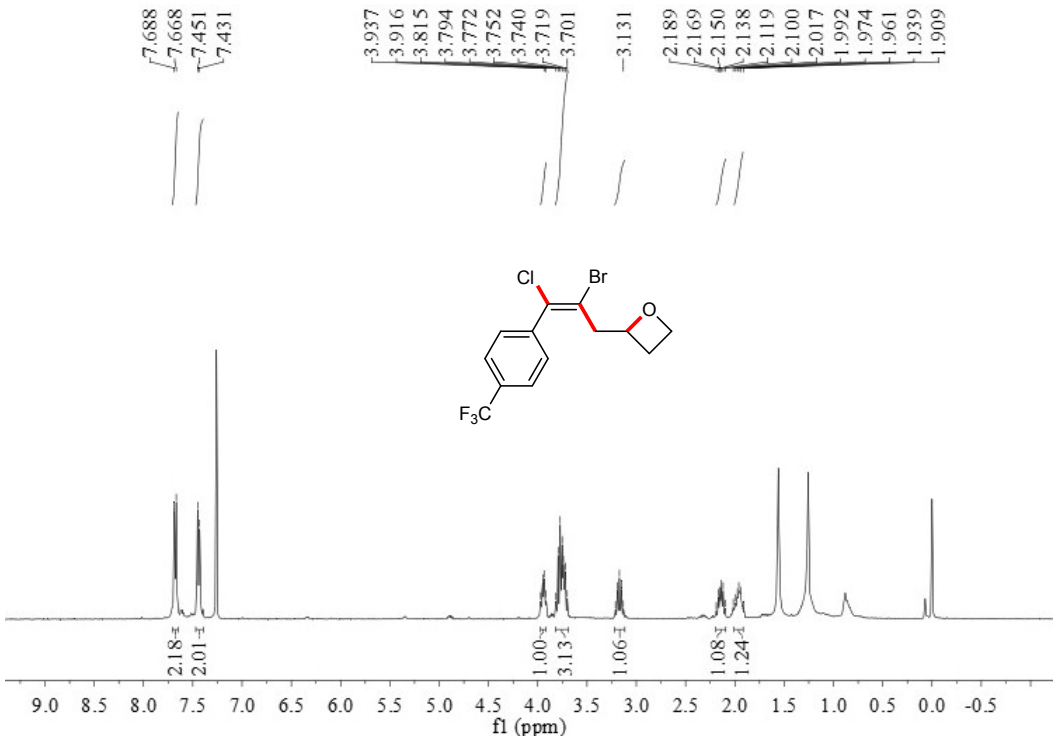
32.691
Cl
Br
O
NC
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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3.740
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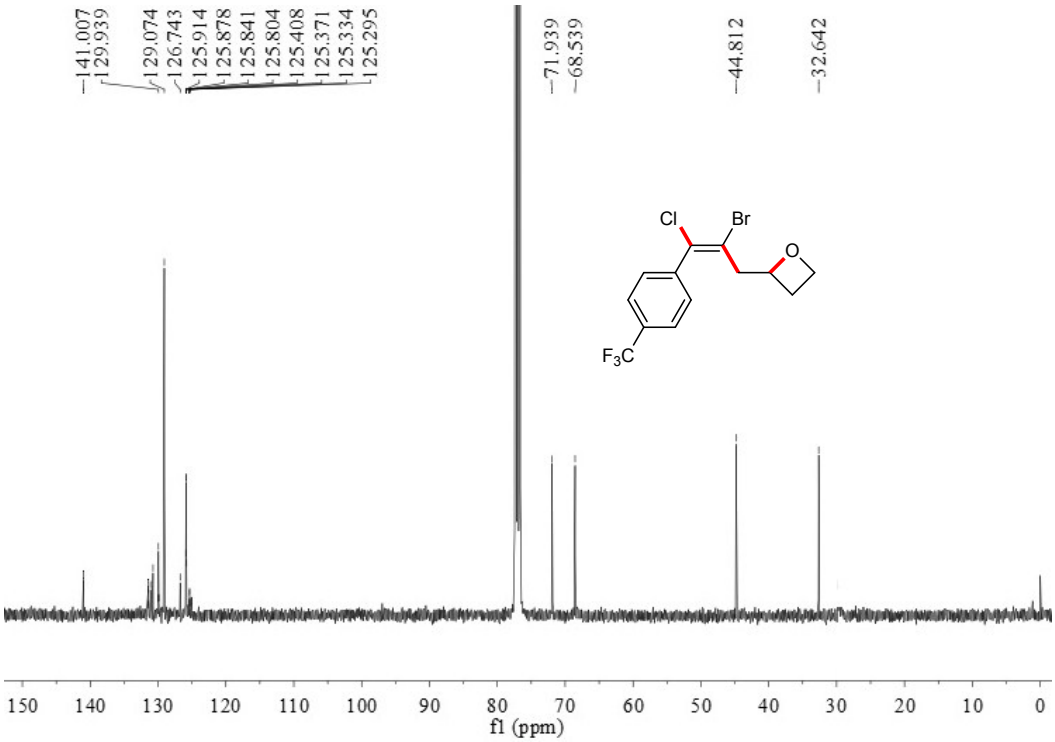
3.701
3.131
2.189
2.169
2.150
2.138
2.119
2.100
2.017
1.992
1.974
1.961
1.939
1.909
Cl
Br
O
F3C
2.18
2.01
1.00
3.13
1.06
1.08
1.24
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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125.804
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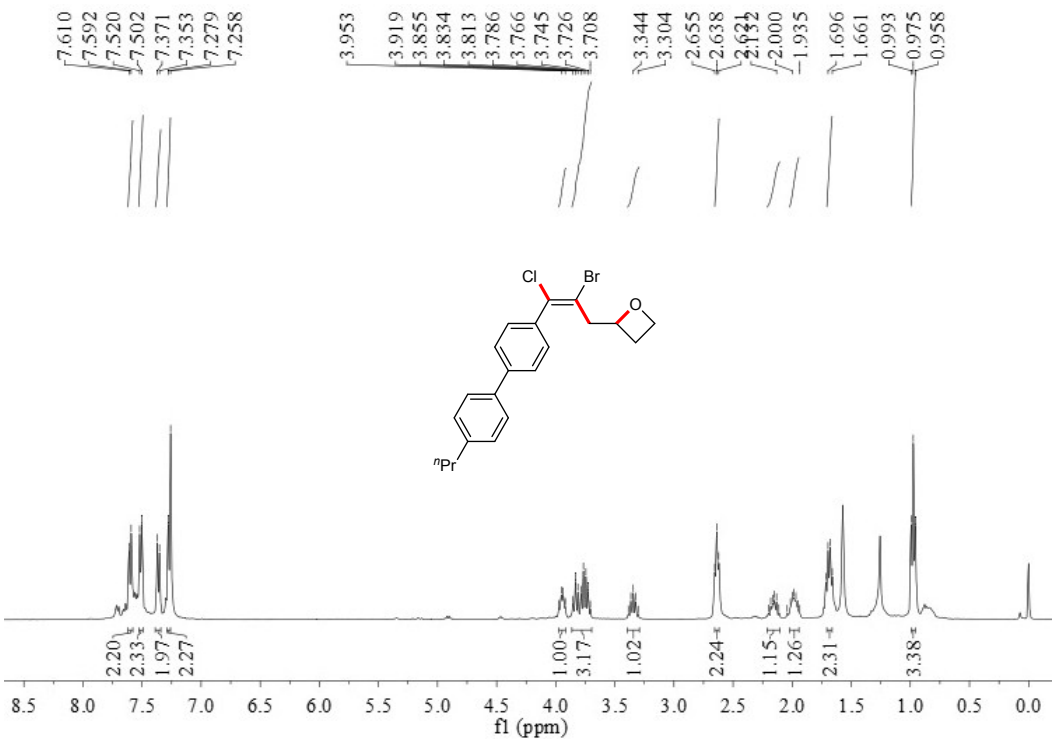
125.371
125.334
125.295
71.939
68.539
44.812
32.642
Cl
Br
O
F3C
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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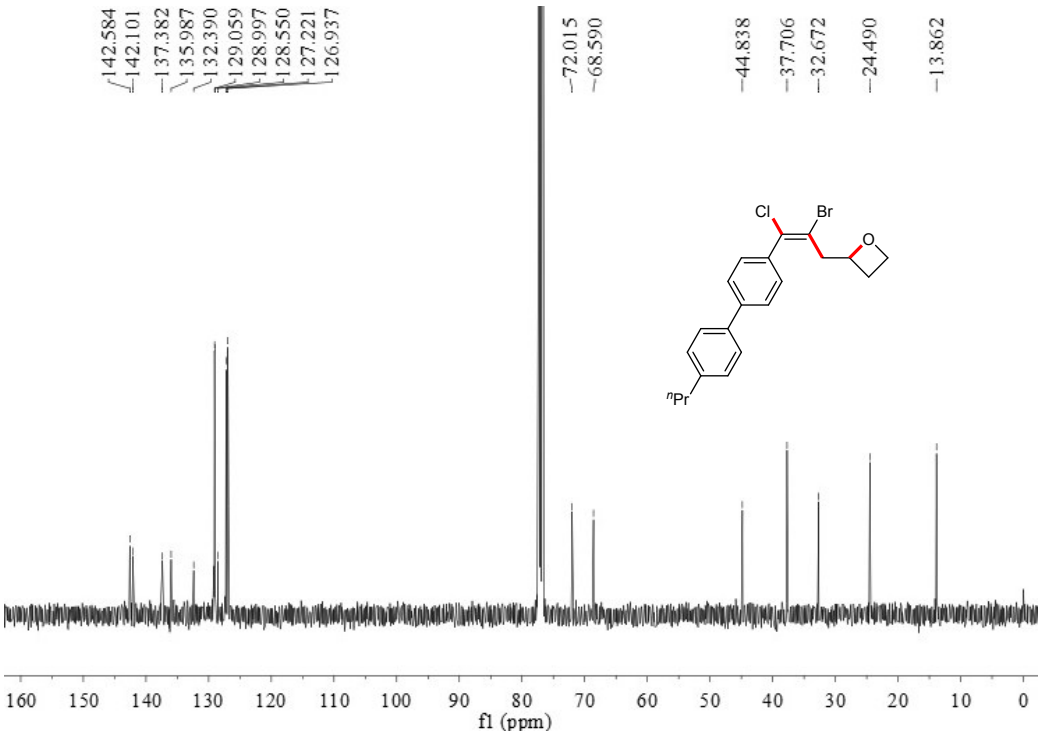
7.592
7.520
7.502
7.371
7.353
7.279
7.258
3.953
3.919
3.855
3.834
3.813
3.786
3.766
3.745
3.726
3.708
3.344
3.304
2.655
2.638
2.621
2.132
2.000
1.935
1.696
1.661
0.993
0.975
0.958
Cl
Br
O
nPr
2.20
2.33
1.97
2.27
1.00
3.17
1.02
2.24
1.15
1.26
2.31
3.38
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.382
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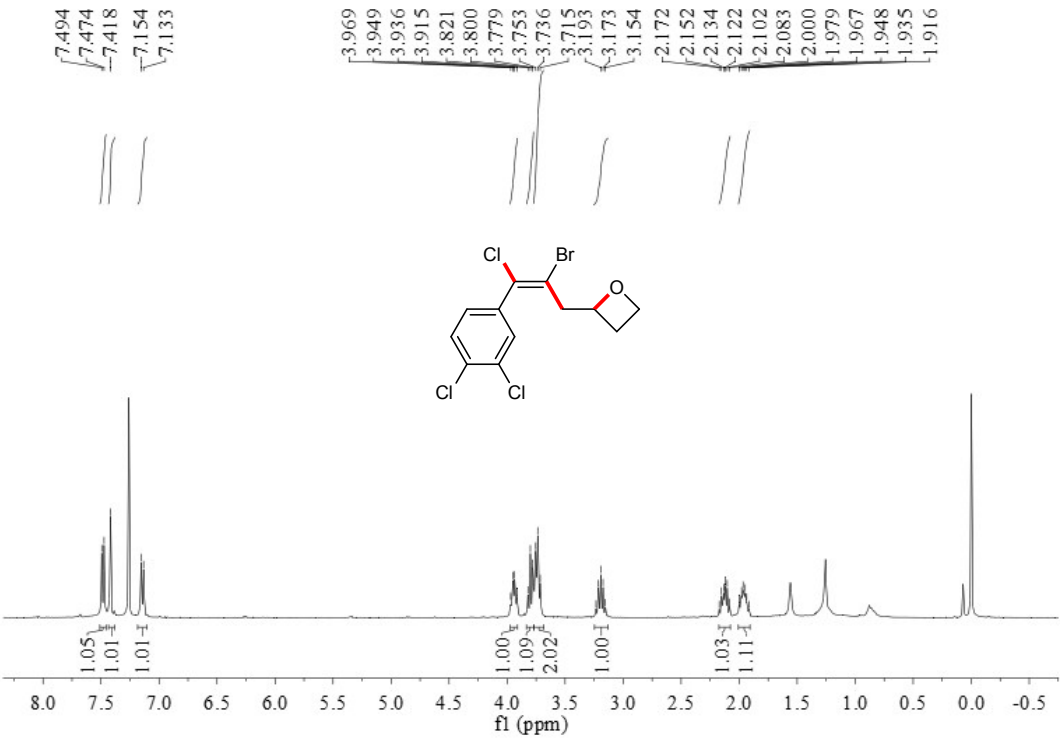
128.997
128.550
127.221
126.937
72.015
68.590
44.838
37.706
32.672
24.490
13.862
Cl
Br
O
nPr
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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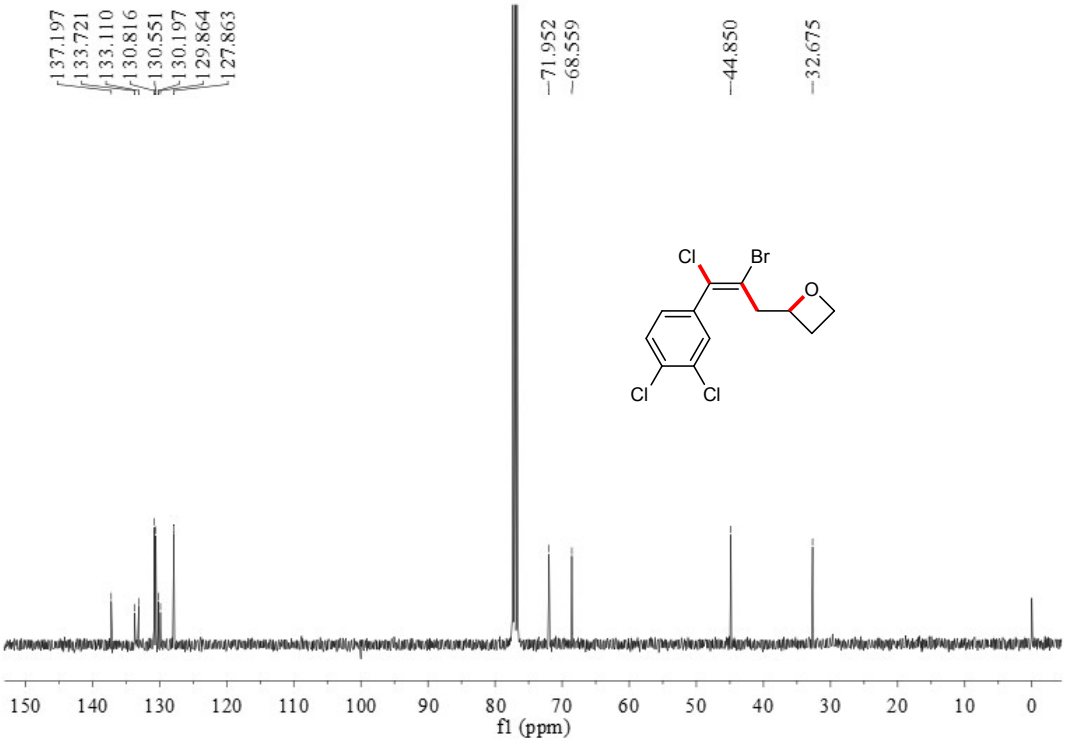
7.474
7.418
7.154
7.133
3.969
3.949
3.936
3.915
3.821
3.800
3.779
3.753
3.736
3.715
3.193
3.173
3.154
2.172
2.152
2.134
2.122
2.102
2.083
2.000
1.979
1.967
1.948
1.935
1.916
Cl
Br
O
Cl
Cl
1.05
1.01
1.01
1.00
1.09
2.02
1.00
1.03
1.11
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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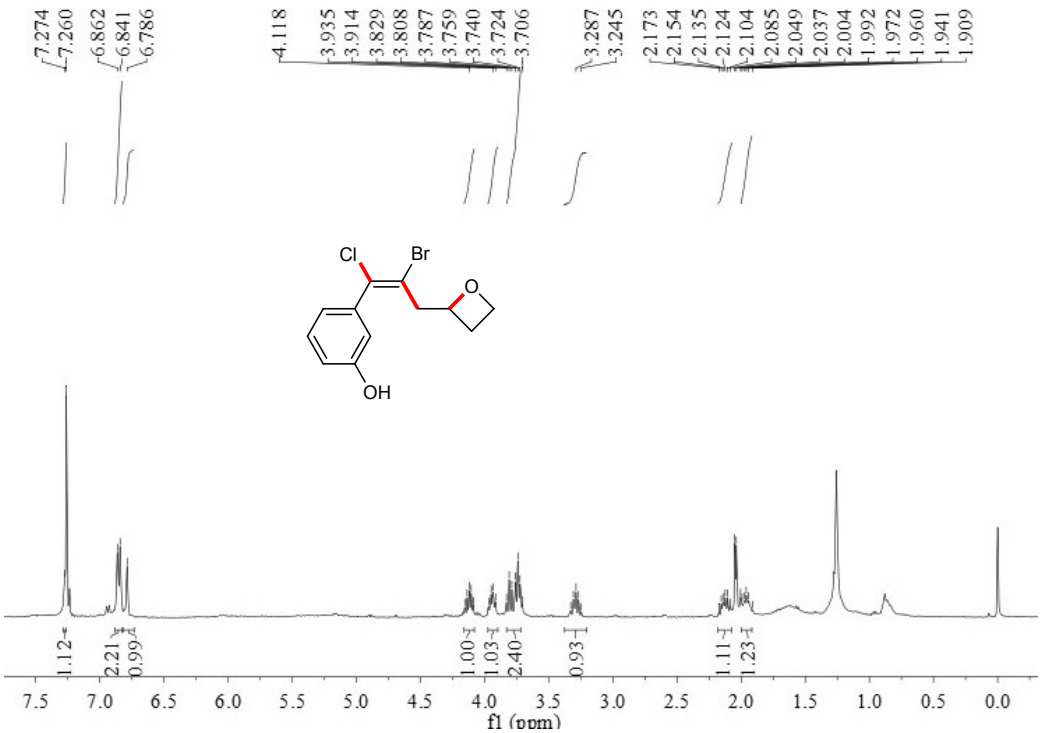
133.721
133.110
130.816
130.551
130.197
129.864
127.863
71.952
68.559
44.850
32.675
Cl
Br
O
Cl
Cl
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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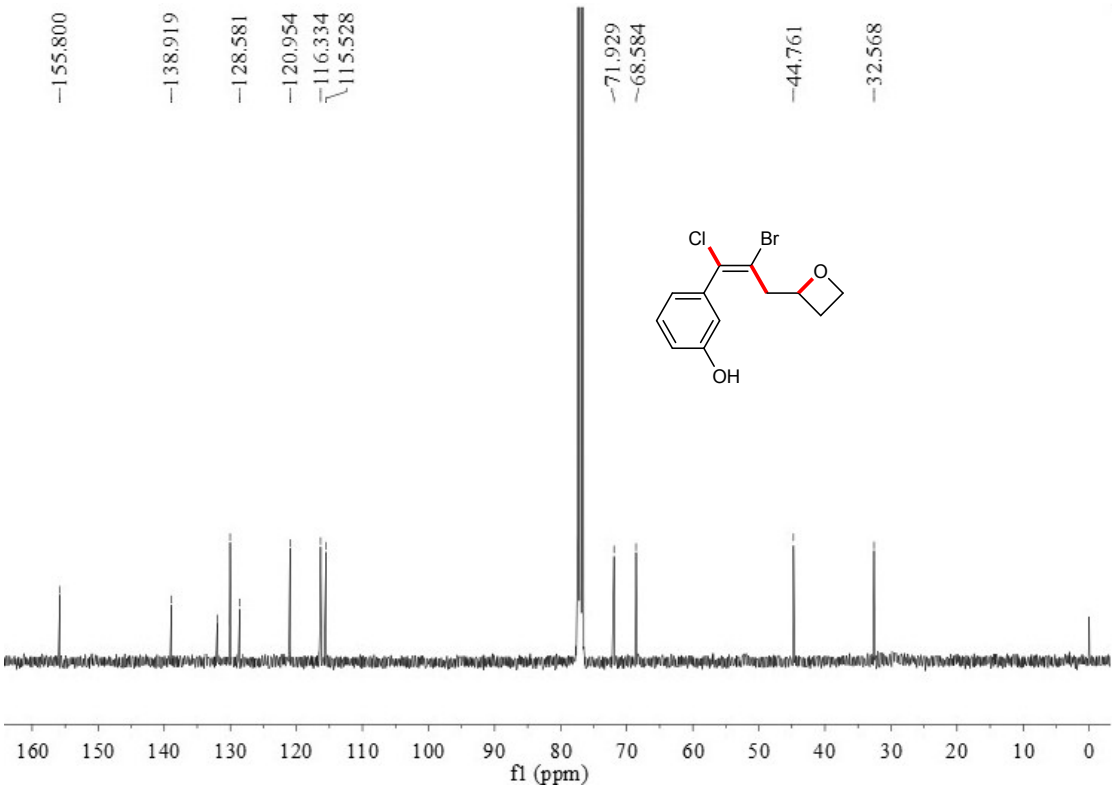
7.260
6.862
6.841
6.786
4.118
3.935
3.914
3.829
3.808
3.787
3.759
3.740
3.724
3.706
3.287
3.245
2.173
2.154
2.135
2.124
2.104
2.085
2.049
2.037
2.004
1.992
1.972
1.960
1.941
1.909
Cl
Br
O
OH
1.12
2.21
0.99
1.00
1.03
2.40
0.93
1.11
1.23
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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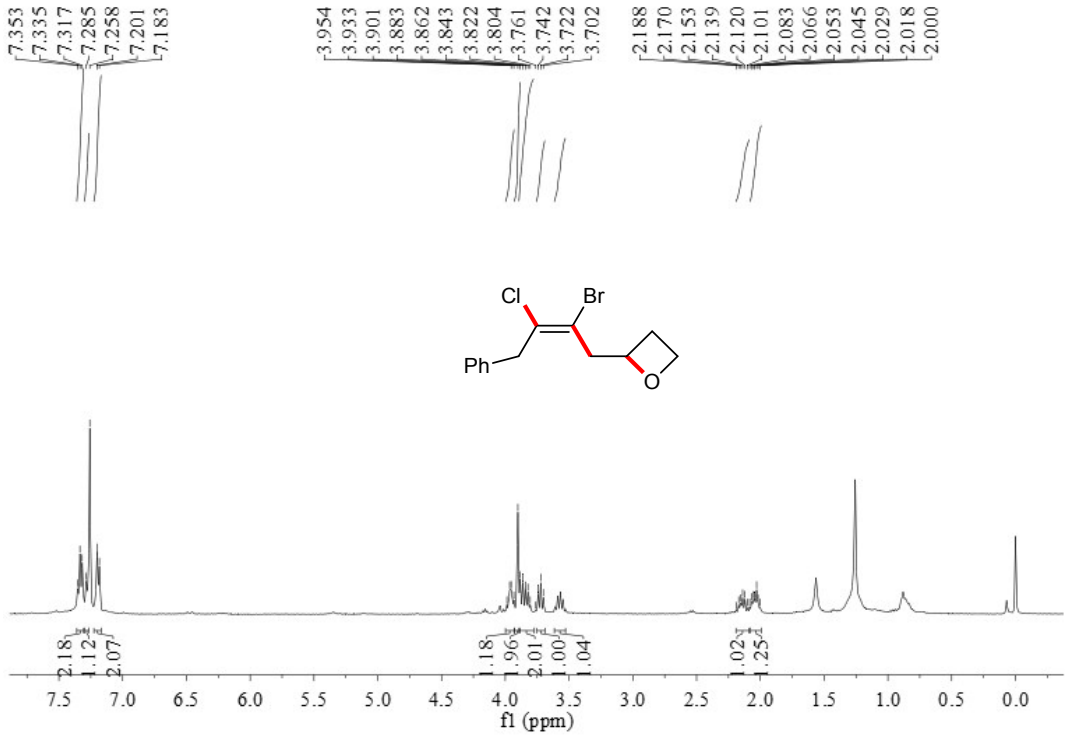
138.919
128.581
120.954
116.334
115.528
71.929
68.584
44.761
32.568
Cl
Br
O
OH
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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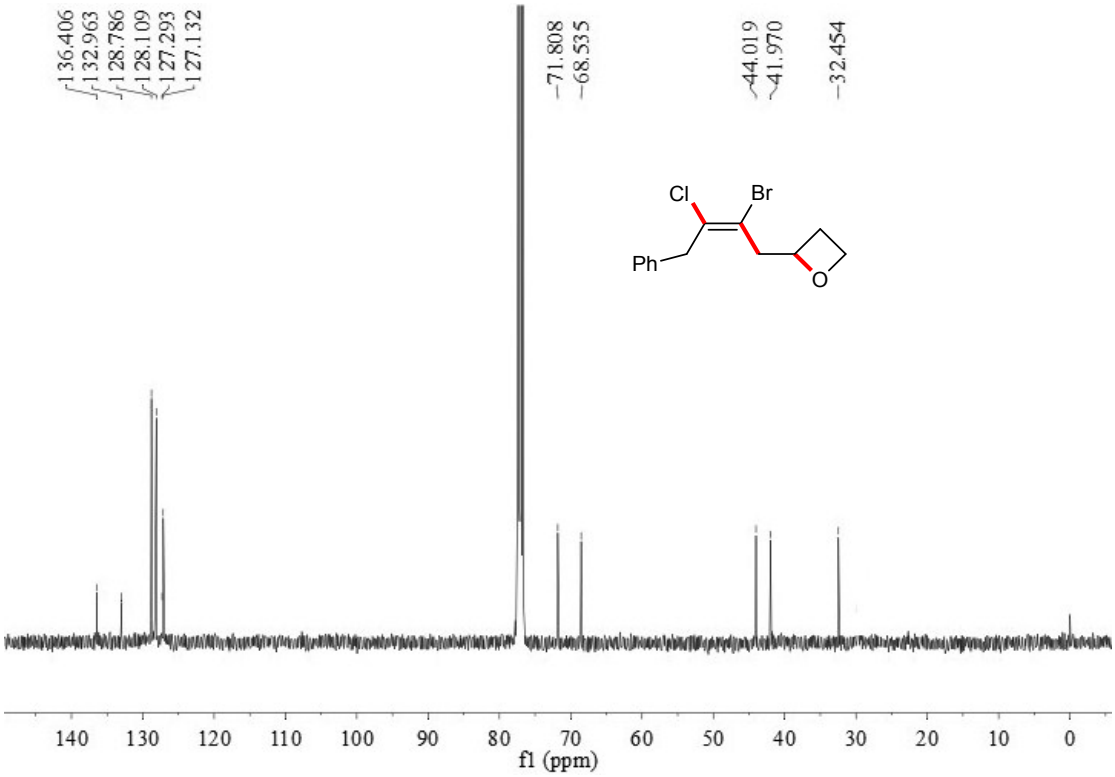
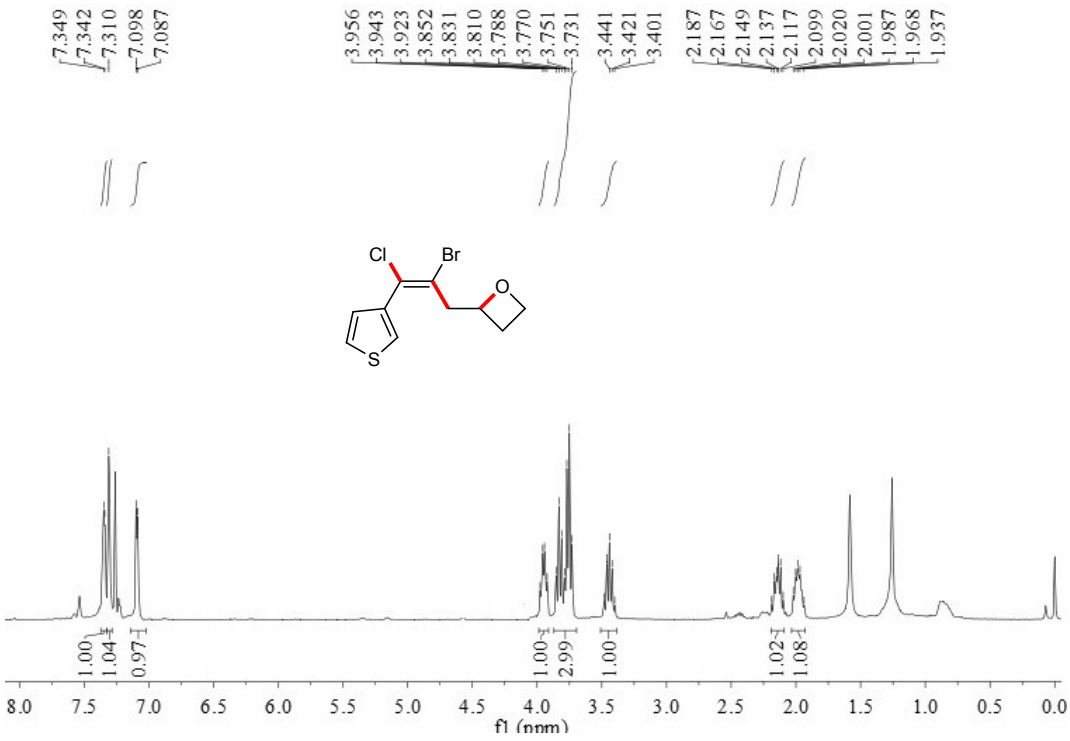
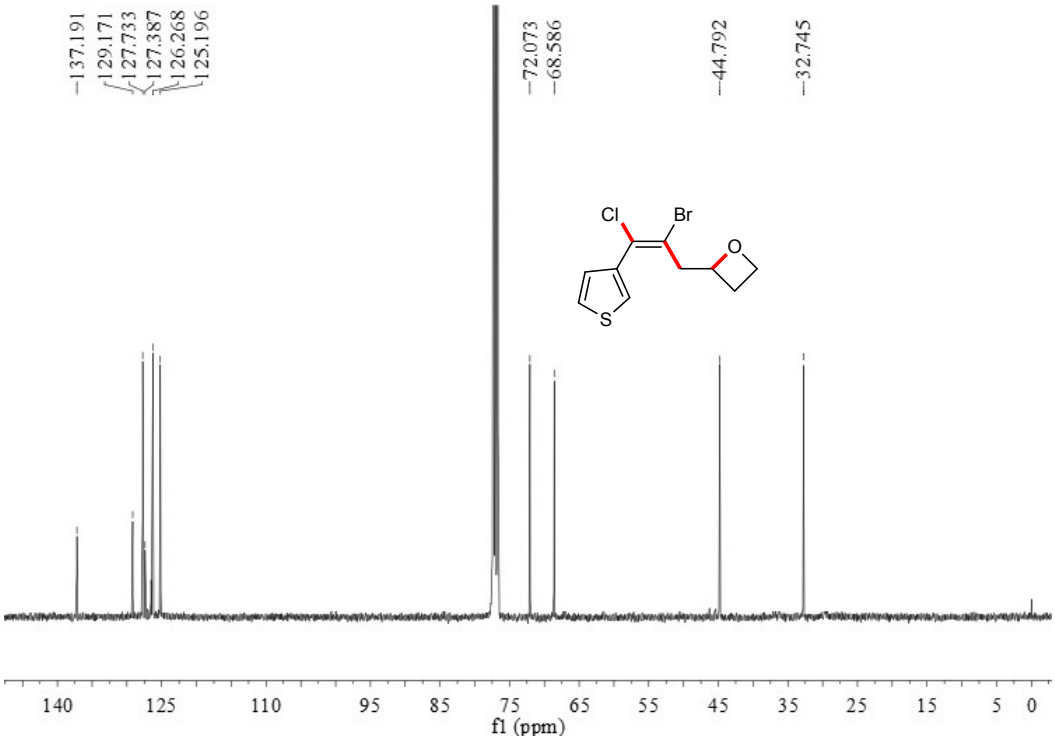
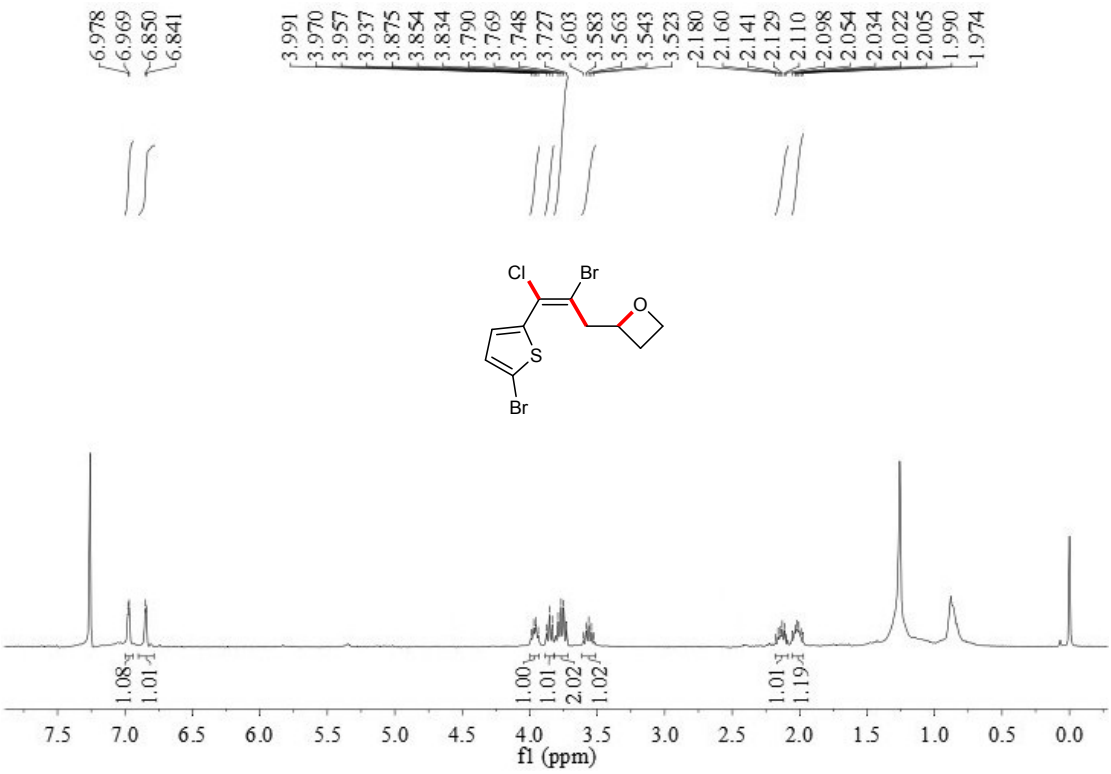
7.285
7.258
7.201
7.183
3.954
3.933
3.901
3.883
3.862
3.843
3.822
3.804
3.761
3.742
3.722
3.702
2.188
2.170
2.153
2.139
2.120
2.101
2.083
2.066
2.053
2.045
2.029
2.018
2.000
Cl
Br
Ph
O
2.18
1.12
2.07
1.18
1.96
2.01
1.00
1.04
1.02
1.25
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


136.406
132.963
128.786
128.109
127.293
127.132
71.808
68.535
44.019
41.970
32.454
Cl
Br
Ph
O
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.349
7.342
7.310
7.098
7.087
3.956
3.943
3.923
3.852
3.831
3.810
3.788
3.770
3.751
3.731
3.441
3.421
3.401
2.187
2.167
2.149
2.137
2.117
2.099
2.020
2.001
1.987
1.968
1.937
Cl
Br
O
S
1.00
1.04
0.97
1.00
2.99
1.00
1.02
1.08
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


137.191
129.171
127.733
127.387
126.268
125.196
72.073
68.586
44.792
32.745
Cl
Br
O
S
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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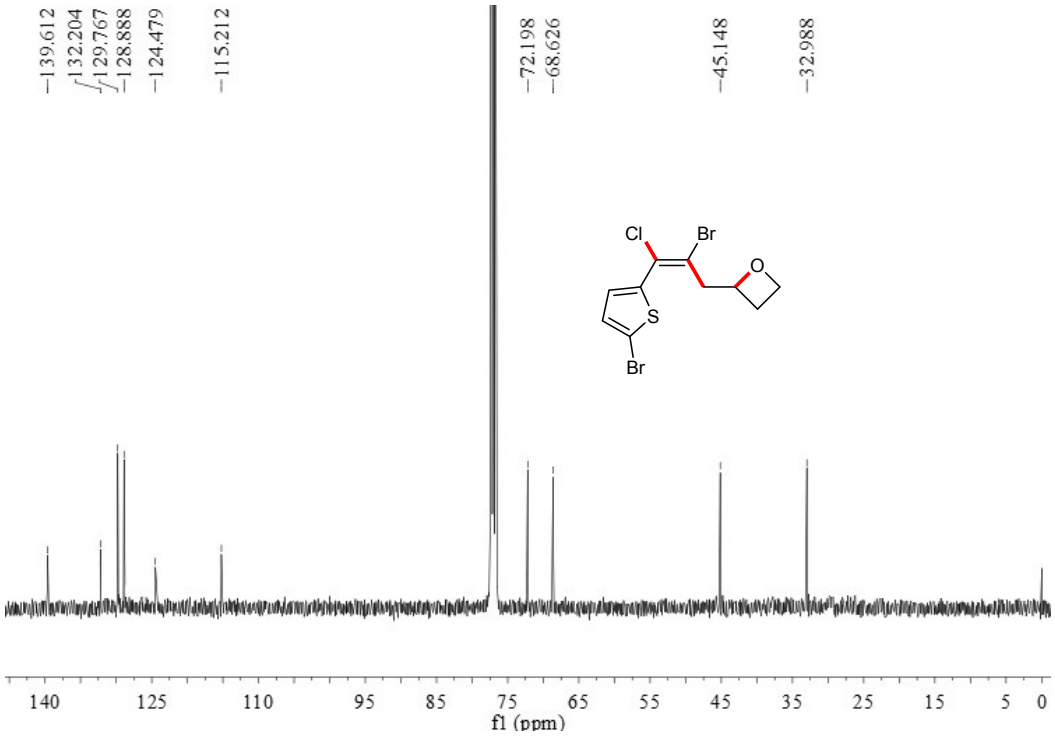
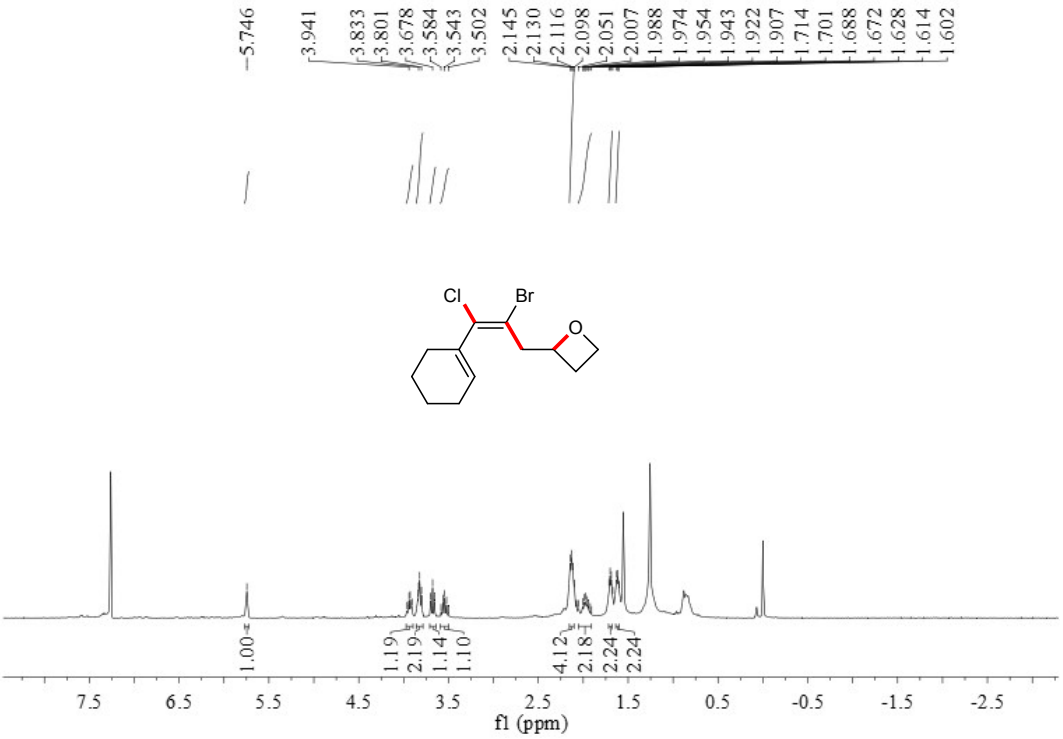
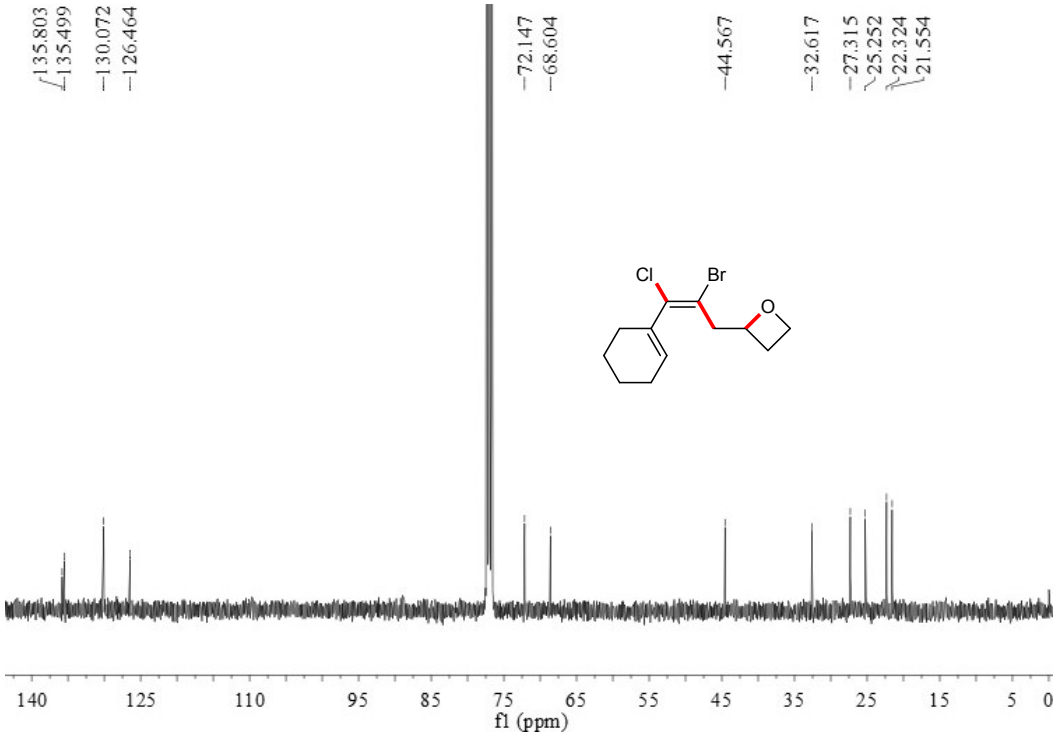
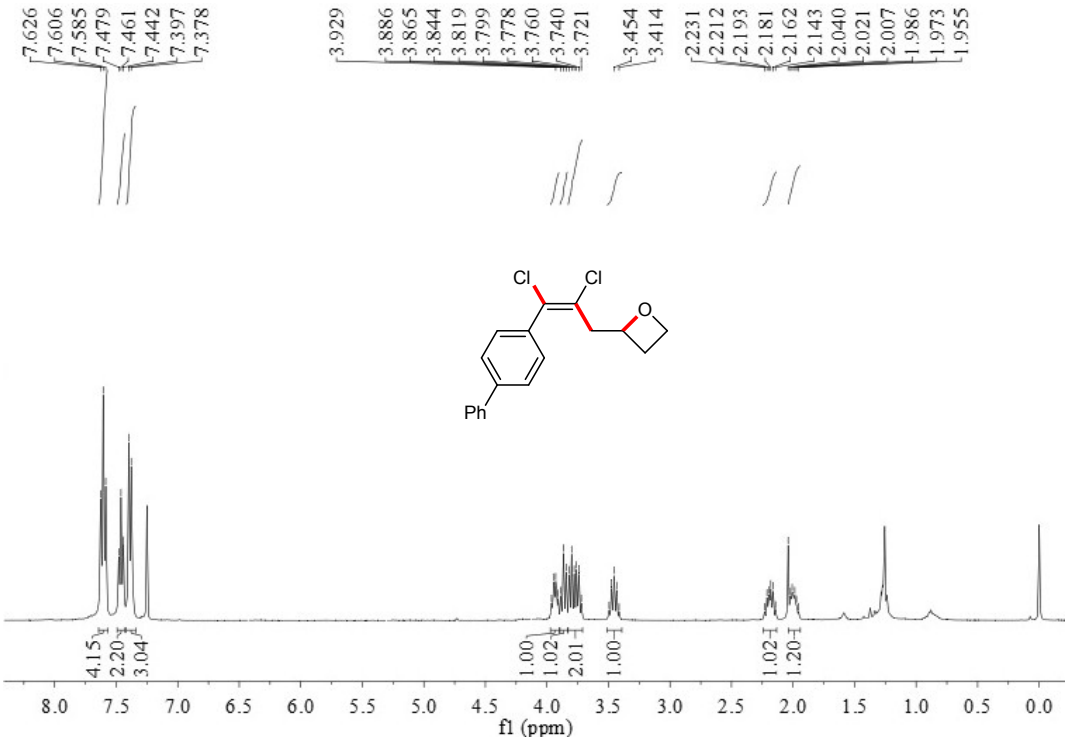
6.969
6.850
6.841
3.991
3.970
3.957
3.937
3.875
3.854
3.834
3.790
3.769
3.748
3.727
3.603
3.583
3.563
3.543
3.523
2.180
2.160
2.141
2.129
2.110
2.098
2.054
2.034
2.022
2.005
1.990
1.974
Cl
Br
O
S
Br
1.08
1.01
1.00
1.01
2.02
1.02
1.01
1.19
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


139.612
132.204
129.767
128.888
124.479
115.212
72.198
68.626
45.148
32.988
Cl
Br
O
S
Br
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)


5.746
3.941
3.833
3.801
3.678
3.584
3.543
3.502
2.145
2.130
2.116
2.098
2.051
2.007
1.988
1.974
1.954
1.943
1.922
1.907
1.714
1.701
1.688
1.672
1.628
1.614
1.602
Cl
Br
O
1.00
1.19
2.19
1.14
1.10
4.12
2.18
2.24
2.24
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
-2.5
f1 (ppm)


135.803
135.499
130.072
126.464
72.147
68.604
44.567
32.617
27.315
25.252
22.324
21.554
Cl
Br
O
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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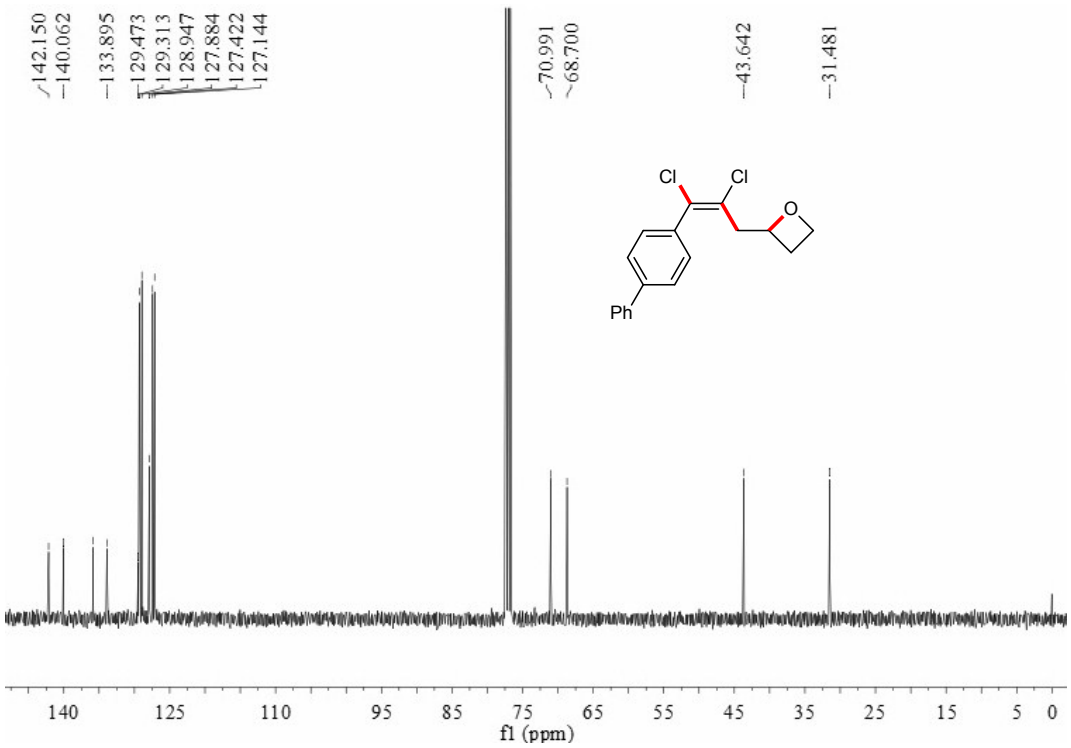
7.479
7.461
7.442
7.397
7.378
3.929
3.886
3.865
3.844
3.819
3.799
3.778
3.760
3.740
3.721
3.454
3.414
2.231
2.212
2.193
2.181
2.162
2.143
2.040
2.021
2.007
1.986
1.973
1.955
Cl
Cl
O
Ph
4.15
2.20
3.04
1.00
1.02
2.01
1.00
1.02
1.20
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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133.895
129.473
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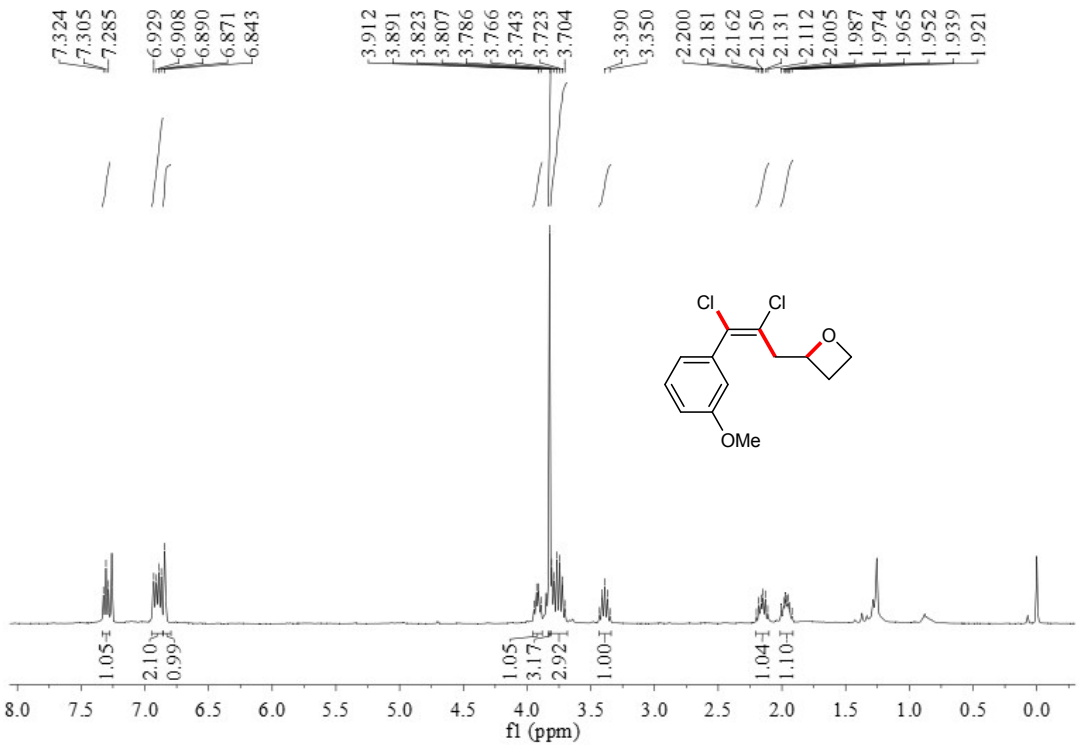
128.947
127.884
127.422
127.144
70.991
68.700
43.642
31.481
Cl
Cl
O
Ph
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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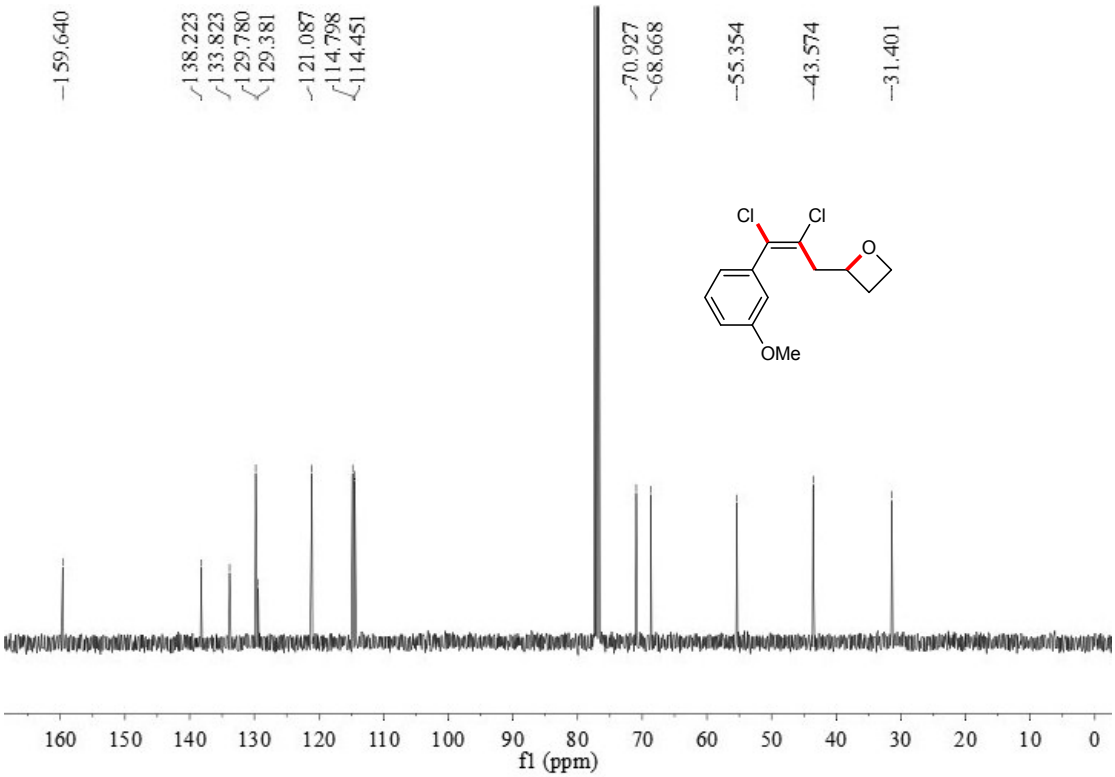
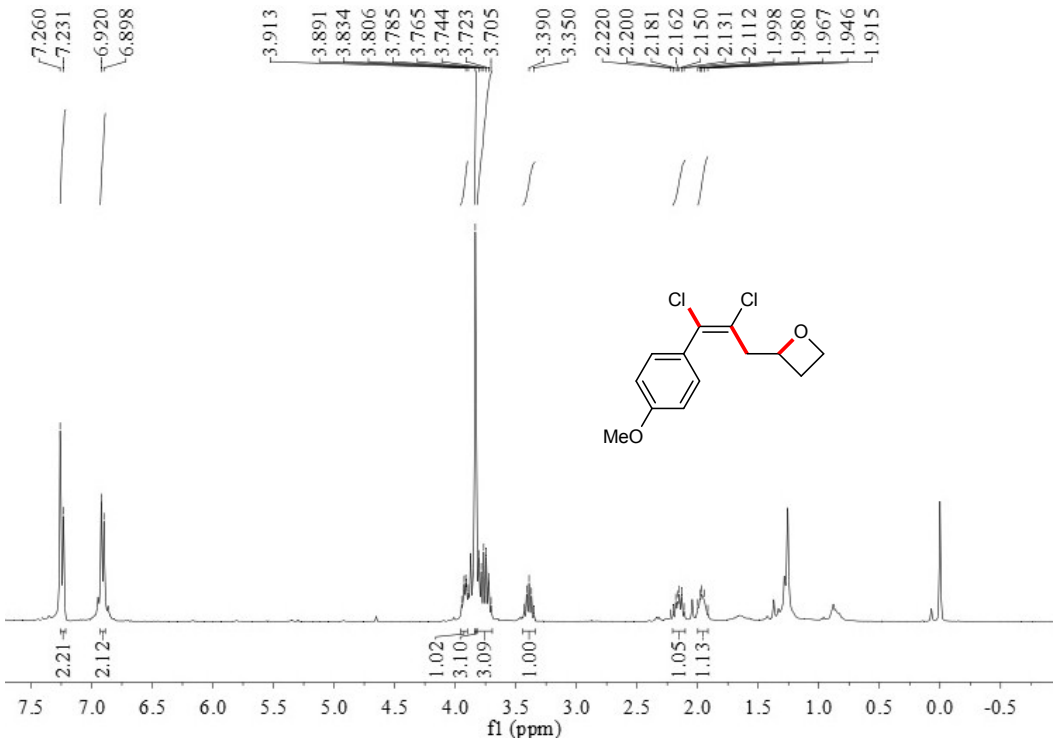
6.908
6.890
6.871
6.843
3.912
3.891
3.823
3.807
3.786
3.766
3.743
3.723
3.704
3.390
3.350
2.200
2.181
2.162
2.150
2.131
2.112
2.005
1.987
1.974
1.965
1.952
1.939
1.921
Cl
Cl
O
OMe
1.05
2.10
0.99
1.05
3.17
2.92
1.00
1.04
1.10
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


159.640
138.223
133.823
129.780
129.381
121.087
114.798
114.451
70.927
68.668
55.354
43.574
31.401
Cl
Cl
O
OMe
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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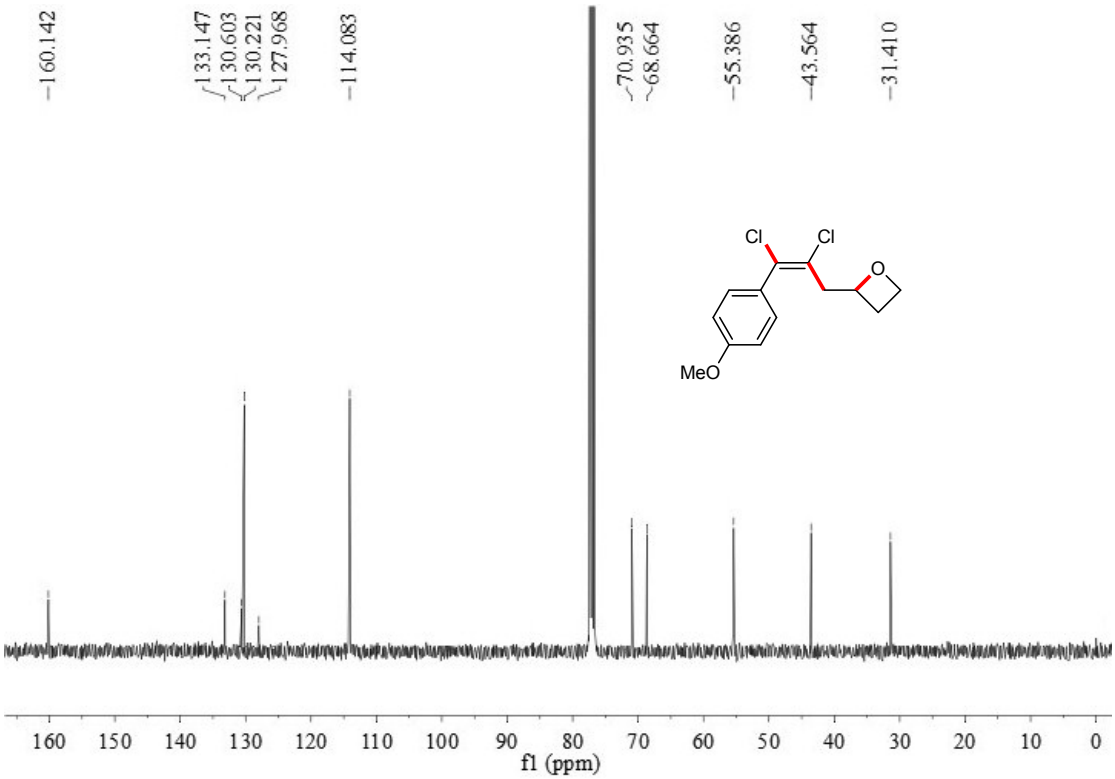
7.231
6.920
6.898
3.913
3.891
3.834
3.806
3.785
3.765
3.744
3.723
3.705
3.390
3.350
2.220
2.200
2.181
2.162
2.150
2.131
2.112
1.998
1.980
1.967
1.946
1.915
Cl
Cl
O
MeO
2.21
2.12
1.02
3.10
3.09
1.00
1.05
1.13
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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130.221
127.968
114.083
70.935
68.664
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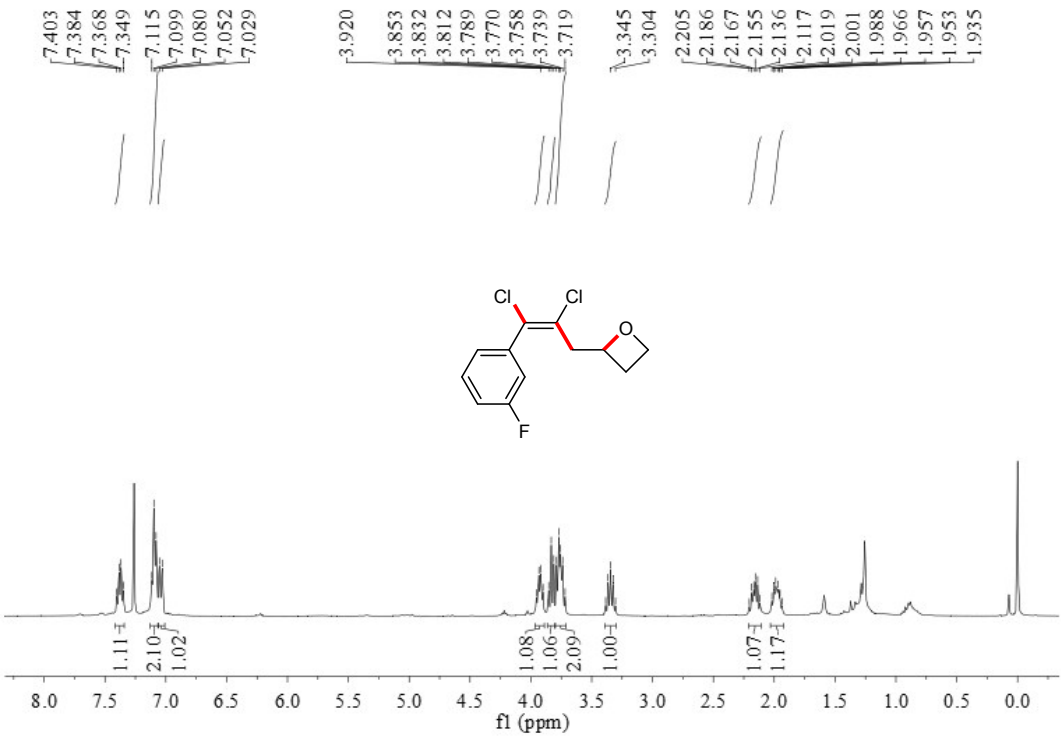
43.564
31.410
Cl
Cl
O
MeO
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.080
7.052
7.029
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3.853
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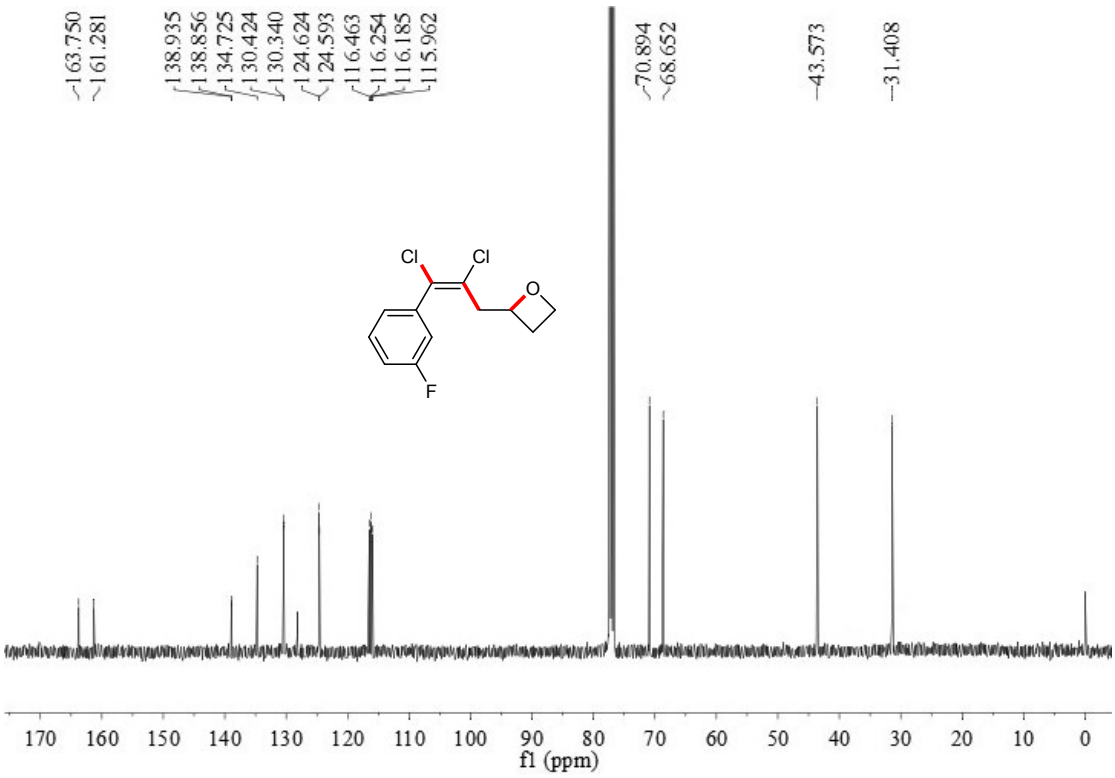
3.812
3.789
3.770
3.758
3.739
3.719
3.345
3.304
2.205
2.186
2.167
2.155
2.136
2.117
2.019
2.001
1.988
1.966
1.957
1.953
1.935
Cl
Cl
O
F
1.11
2.10
1.02
1.08
1.06
2.09
1.00
1.07
1.17
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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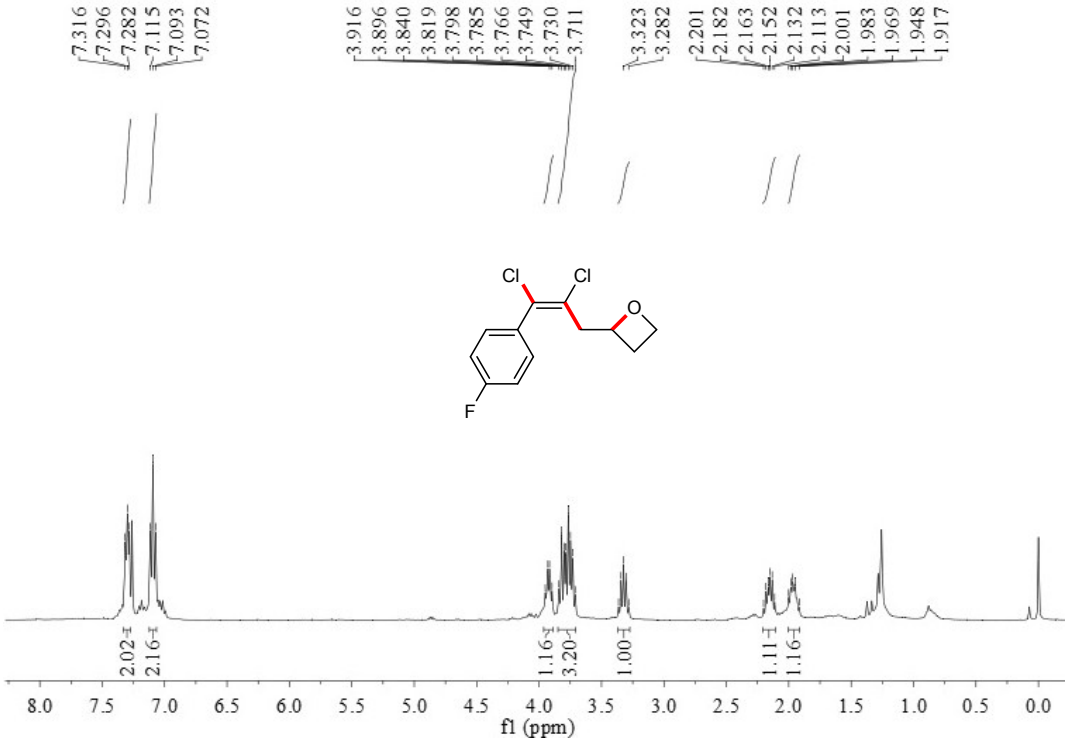
161.281
138.935
138.856
134.725
130.424
130.340
124.624
124.593
116.463
116.254
116.185
115.962
70.894
68.652
43.573
31.408
Cl
Cl
O
F
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.316
7.296
7.282
7.115
7.093
7.072
3.916
3.896
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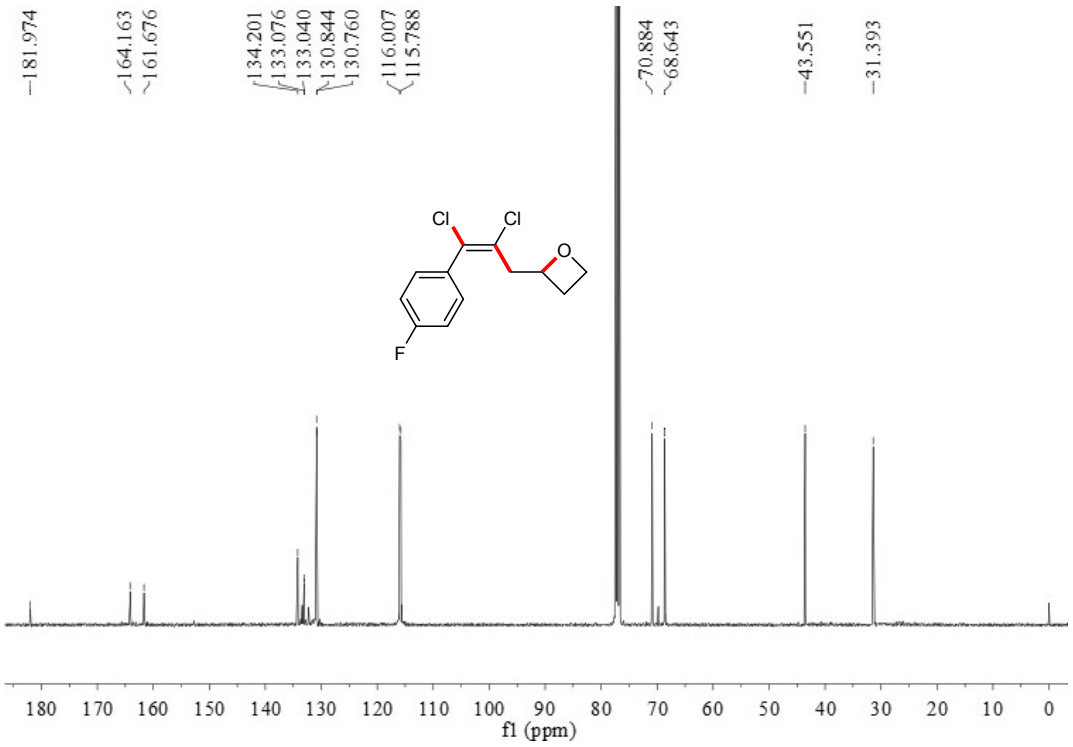
3.819
3.798
3.785
3.766
3.749
3.730
3.711
3.323
3.282
2.201
2.182
2.163
2.152
2.132
2.113
2.001
1.983
1.969
1.948
1.917
Cl
Cl
O
F
2.02
2.16
1.16
3.20
1.00
1.11
1.16
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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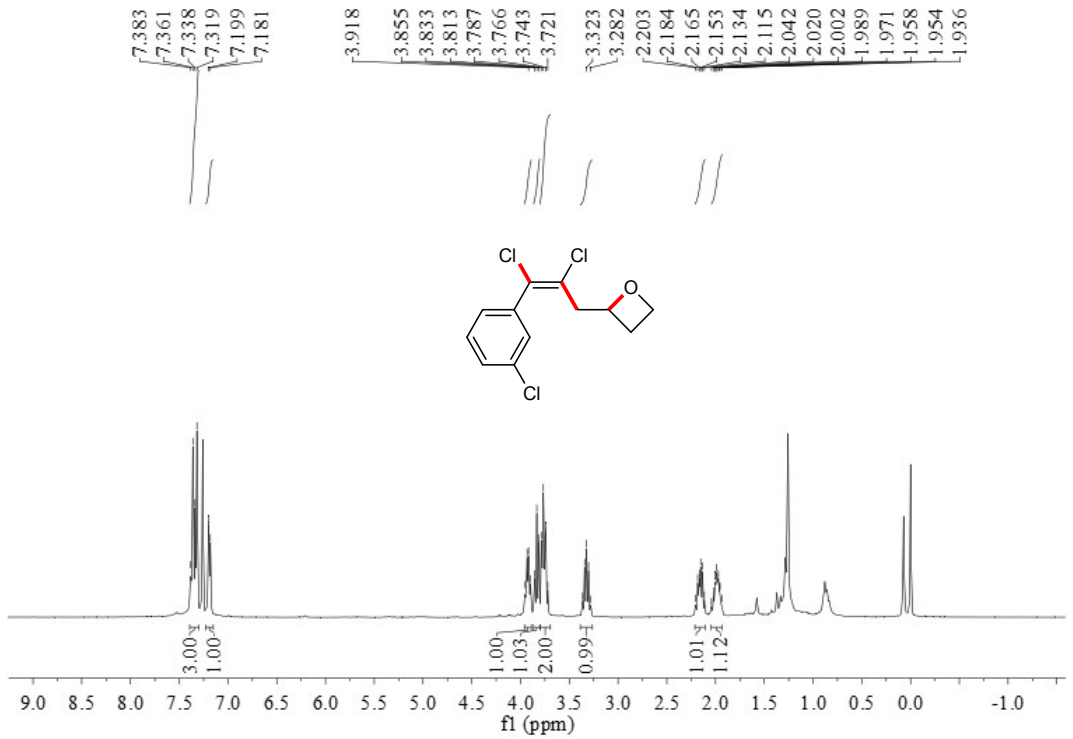
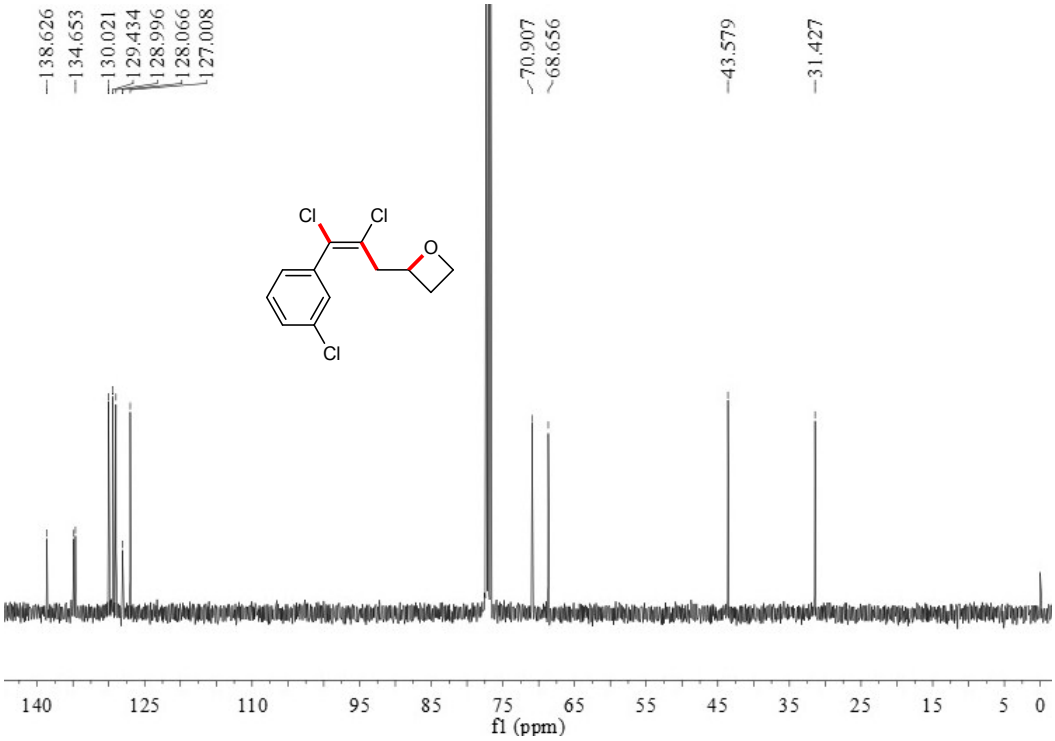
161.676
134.201
133.076
133.040
130.844
130.760
116.007
115.788
70.884
68.643
43.551
31.393
Cl
Cl
O
F
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.383
7.361
7.338
7.319
7.199
7.181
3.918
3.855
3.833
3.813
3.787
3.766
3.743
3.721
3.323
3.282
2.203
2.184
2.165
2.153
2.134
2.115
2.042
2.020
2.002
1.989
1.971
1.958
1.954
1.936
Cl
Cl
O
Cl
3.00
1.00
1.00
1.03
2.00
0.99
1.01
1.12
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0
f1 (ppm)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134.653
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70.907
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43.579
31.427
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Cl
O
Cl
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125
110
95
85
75
65
55
45
35
25
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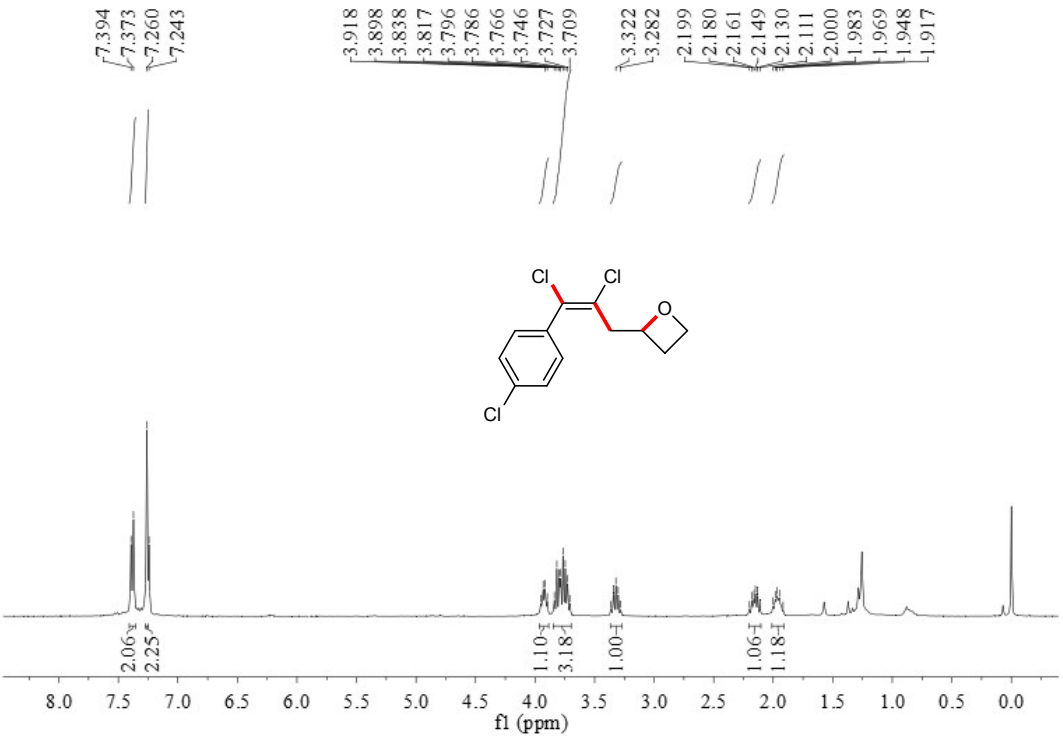
0
f1 (ppm)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3.817
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3.766
3.746
3.727
3.709
3.322
3.282
2.199
2.180
2.161
2.149
2.130
2.111
2.000
1.983
1.969
1.948
1.917
Cl
Cl
O
Cl
2.06
2.25
1.10
3.18
1.00
1.06
1.18
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
1.5
1.0
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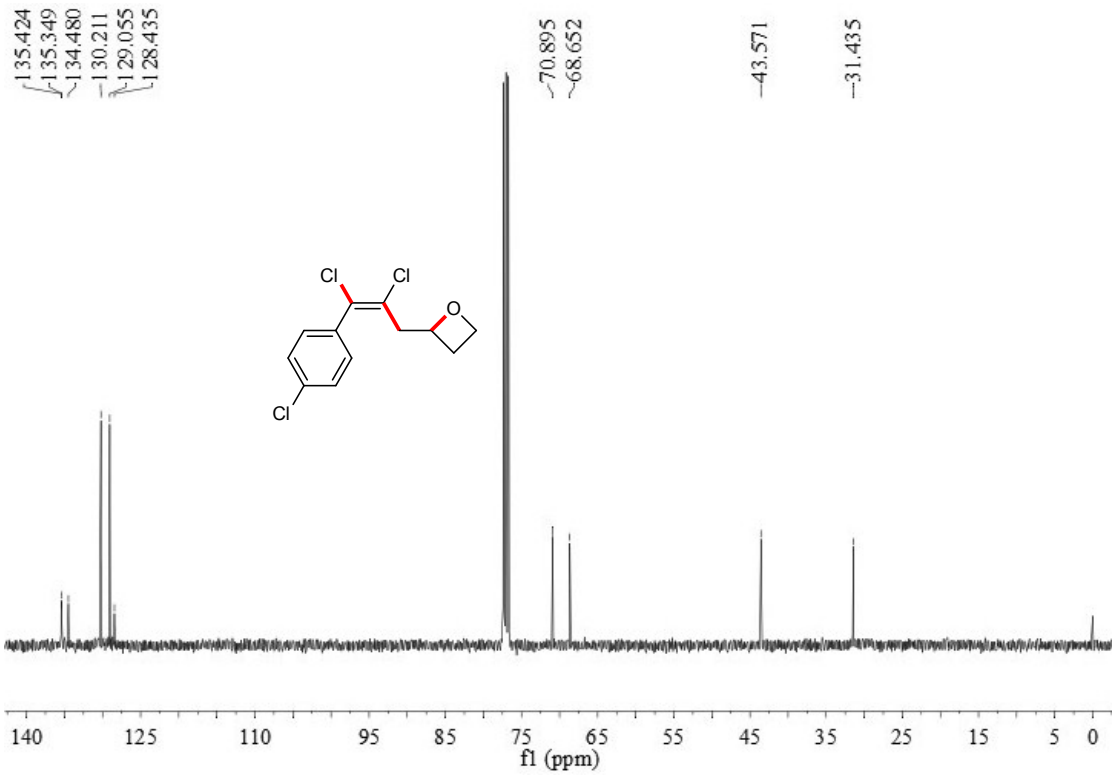
0.0
f1 (ppm)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135.349
134.480
130.211
129.055
128.435
70.895
68.652
43.571
31.435
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Cl
O
Cl
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125
110
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85
75
65
55
45
35
25
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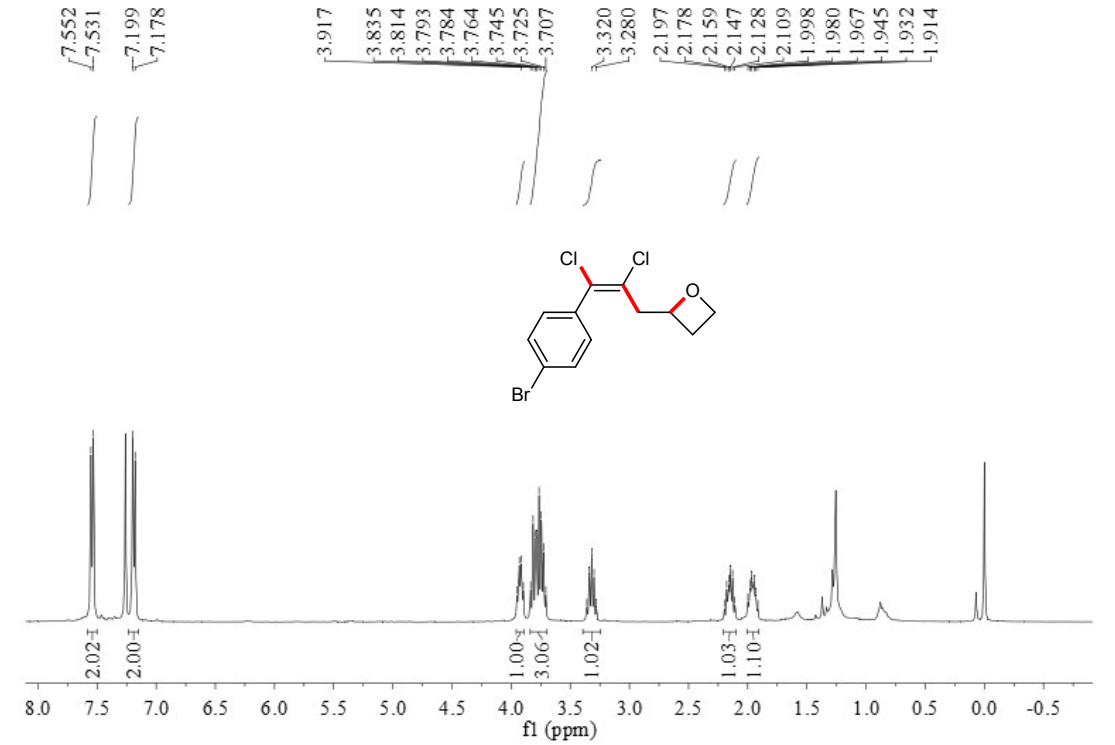
0
f1 (ppm)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7.199
7.178
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3.835
3.814
3.793
3.784
3.764
3.745
3.725
3.707
3.320
3.280
2.197
2.178
2.159
2.147
2.128
2.109
1.998
1.980
1.967
1.945
1.932
1.914
Cl
Cl
O
Br
2.02
2.00
1.00
3.06
1.02
1.03
1.10
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
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3.0
2.5
2.0
1.5
1.0
0.5
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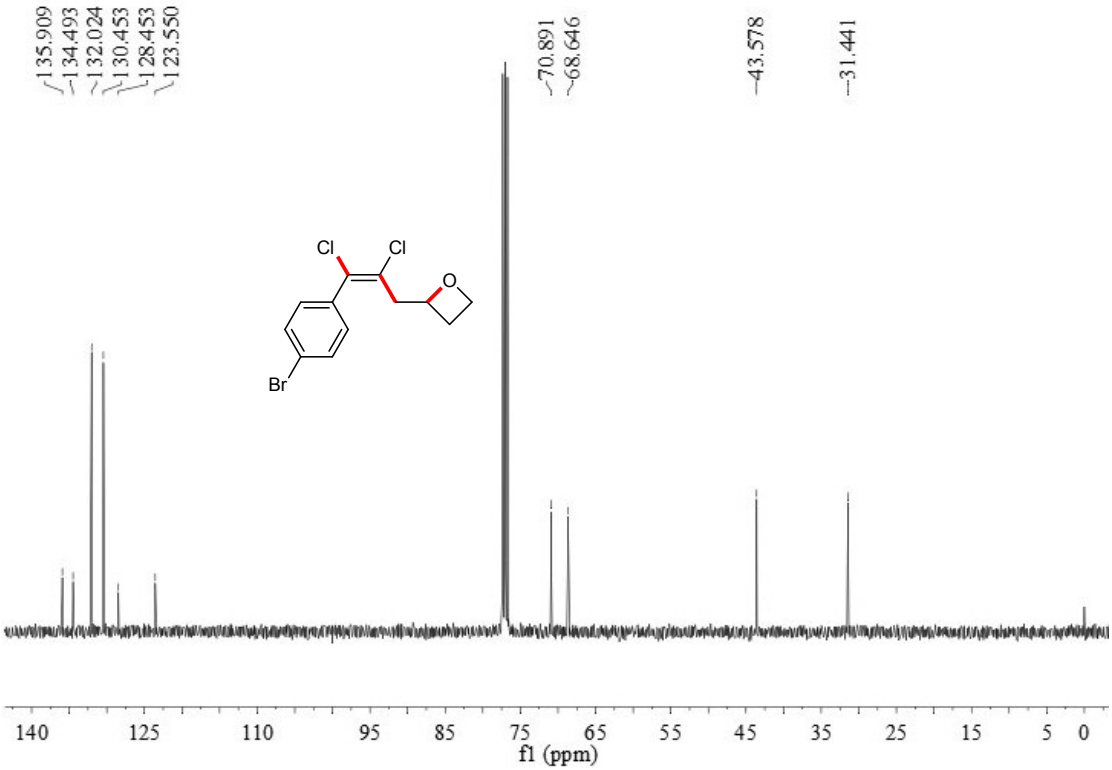
-0.5
f1 (ppm)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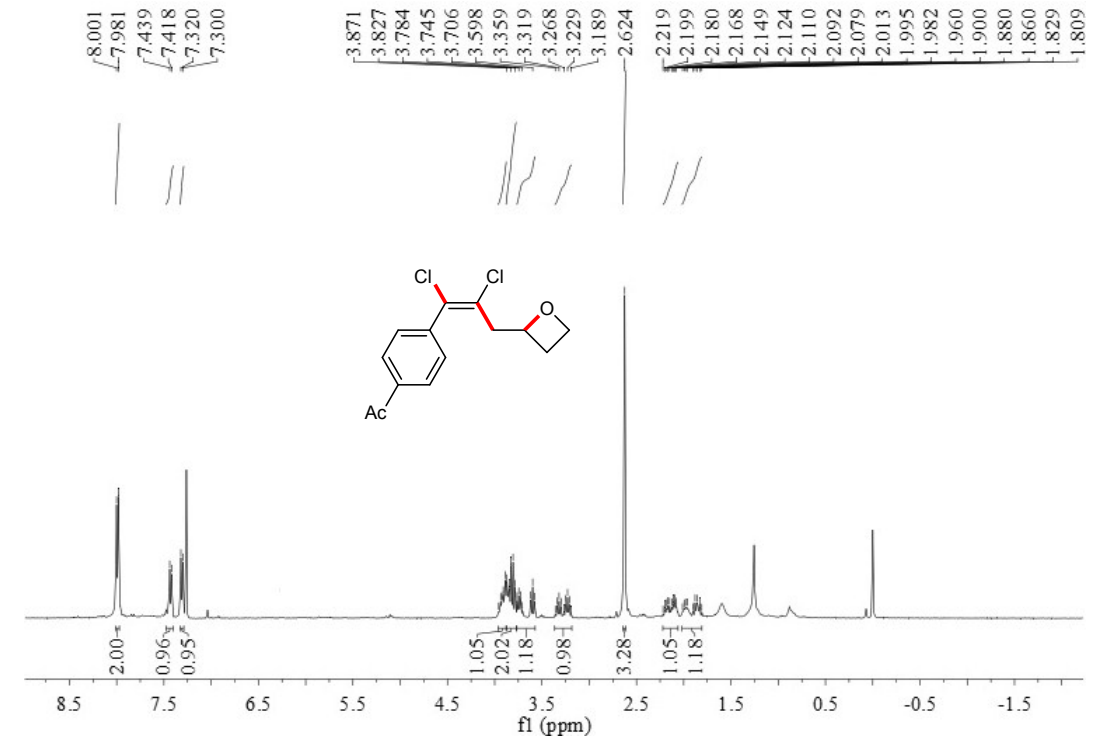
132.024
130.453
128.453
123.550
70.891
68.646
43.578
31.441
Cl
Cl
O
Br
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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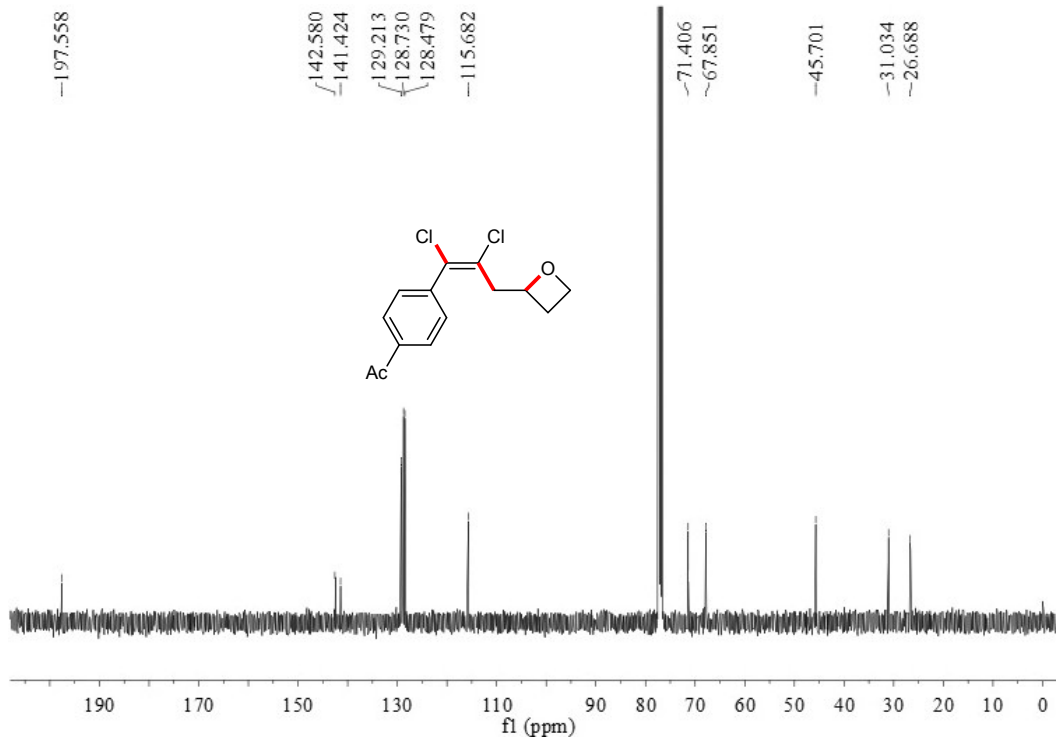
3.871
3.827
3.784
3.745
3.706
3.598
3.359
3.319
3.268
3.229
3.189
2.624
2.219
2.199
2.180
2.168
2.149
2.124
2.110
2.092
2.079
2.013
1.995
1.982
1.960
1.900
1.880
1.860
1.829
1.809
Cl
Cl
O
Ac
2.00
0.96
0.95
1.05
2.02
1.18
0.98
3.28
1.05
1.18
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)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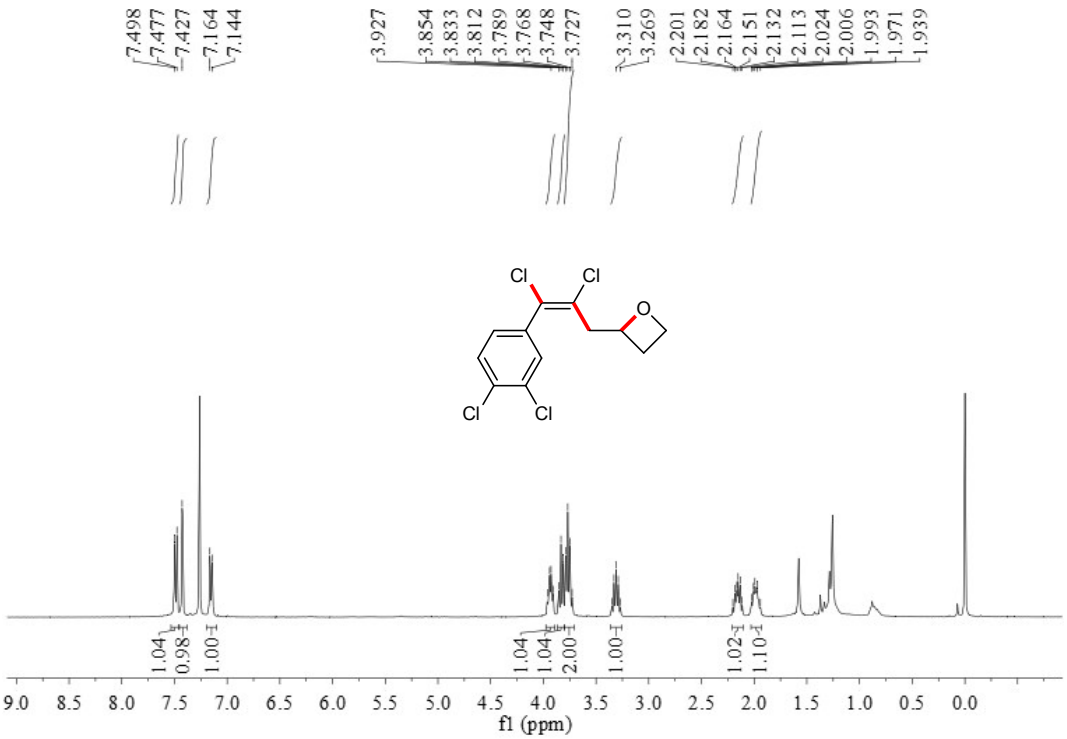
141.424
129.213
128.730
128.479
115.682
71.406
67.851
45.701
31.034
26.688
Cl
Cl
O
Ac
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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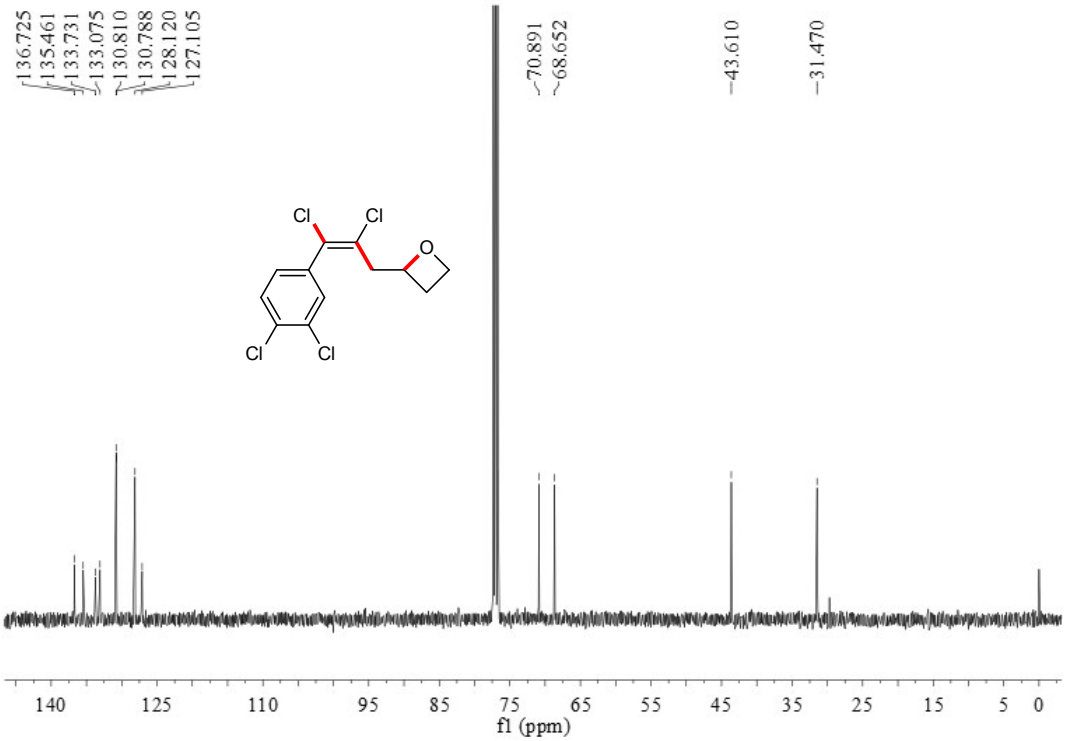
7.427
7.164
7.144
3.927
3.854
3.833
3.812
3.789
3.768
3.748
3.727
3.310
3.269
2.201
2.182
2.164
2.151
2.132
2.113
2.024
2.006
1.993
1.971
1.939
Cl
Cl
O
Cl
Cl
1.04
0.98
1.00
1.04
1.04
2.00
1.00
1.02
1.10
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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133.731
133.075
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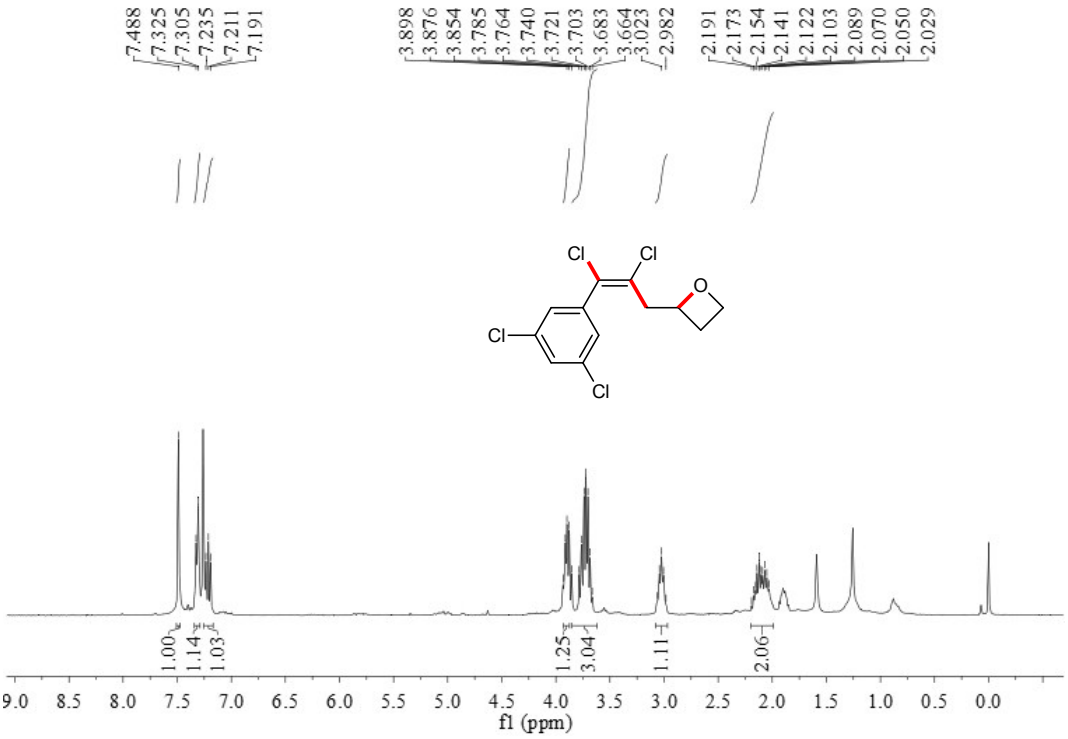
130.788
128.120
127.105
70.891
68.652
43.610
31.470
Cl
Cl
O
Cl
Cl
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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3.854
3.785
3.764
3.740
3.721
3.703
3.683
3.664
3.023
2.982
2.191
2.173
2.154
2.141
2.122
2.103
2.089
2.070
2.050
2.029
Cl
Cl
O
Cl
Cl
1.00
1.14
1.03
1.25
3.04
1.11
2.06
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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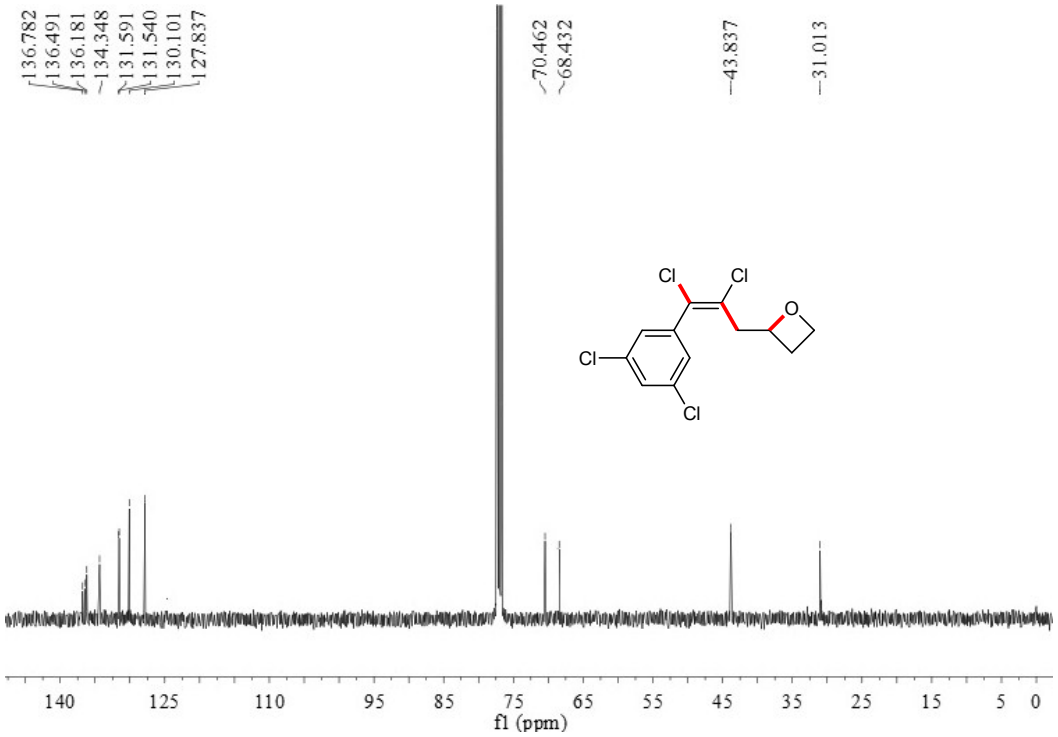
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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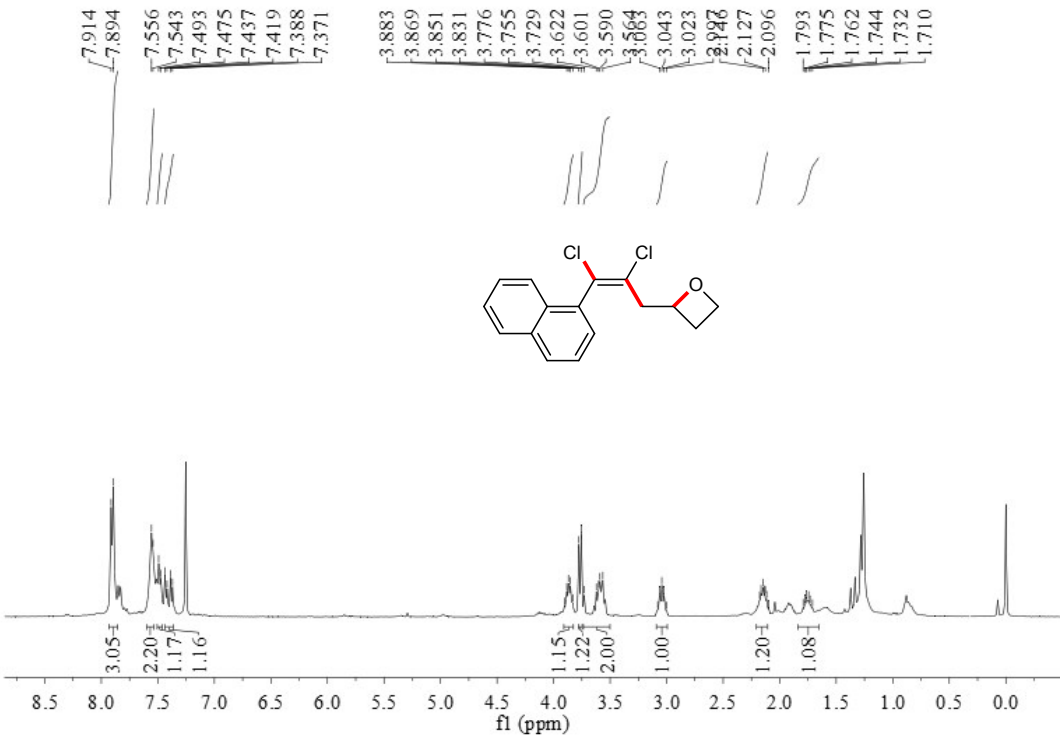
136.181
134.348
131.591
131.540
130.101
127.837
70.462
68.432
43.837
31.013
Cl
Cl
Cl
Cl
O
140
125
110
95
85
75
65
55
45
35
25
15
5
0
f1 (ppm)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3.883
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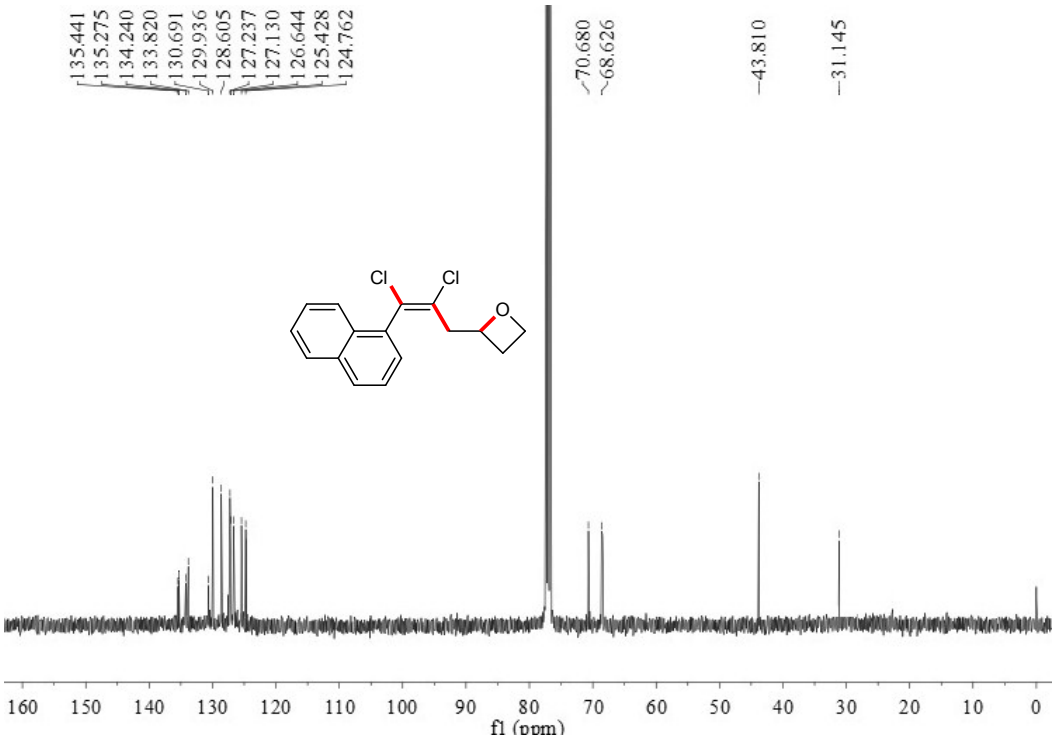
3.851
3.831
3.776
3.755
3.729
3.622
3.601
3.590
3.043
3.023
2.127
2.096
1.793
1.775
1.762
1.744
1.732
1.710
Cl
Cl
O
3.05
2.20
1.17
1.16
1.15
1.22
2.00
1.00
1.20
1.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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129.936
128.605
127.237
127.130
126.644
125.428
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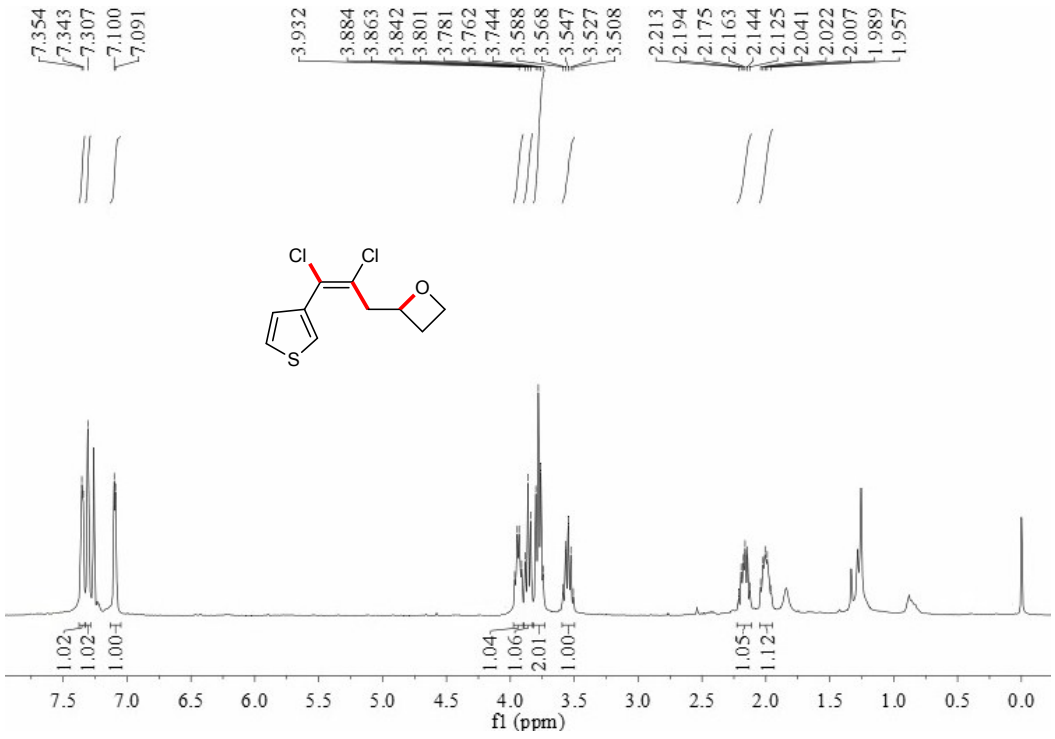
68.626
43.810
31.145
Cl
Cl
O
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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3.781
3.762
3.744
3.588
3.568
3.547
3.527
3.508
2.213
2.194
2.175
2.163
2.144
2.125
2.041
2.022
2.007
1.989
1.957
Cl
Cl
O
S
1.02
1.02
1.00
1.04
1.06
2.01
1.00
1.05
1.12
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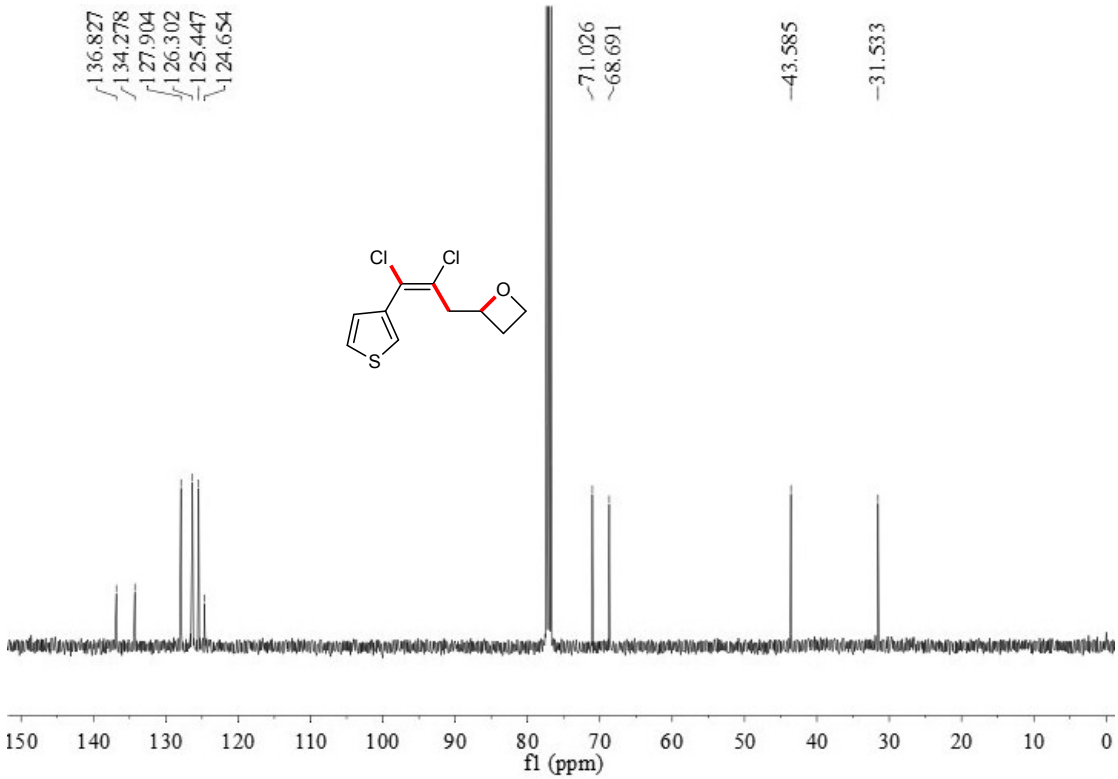
f1 (ppm)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O
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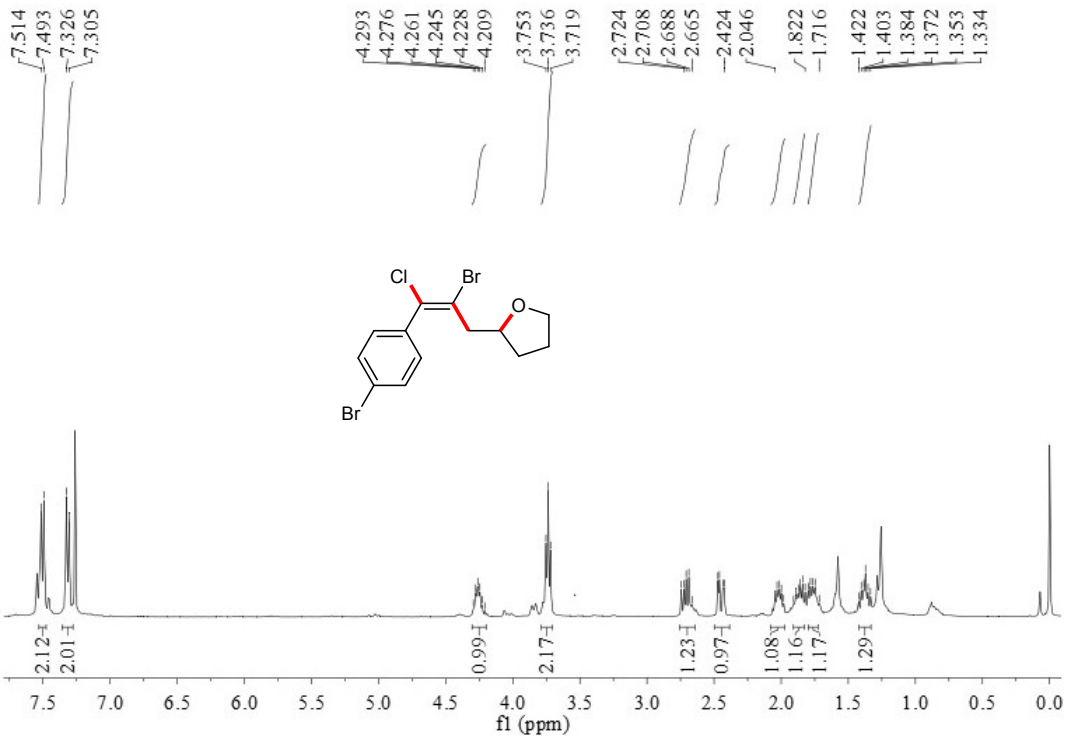
f1 (ppm)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4.245
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4.209
3.753
3.736
3.719
2.724
2.708
2.688
2.665
2.424
2.046
1.822
1.716
1.422
1.403
1.384
1.372
1.353
1.334
Cl
Br
O
Br
2.12
2.01
0.99
2.17
1.23
0.97
1.08
1.16
1.17
1.29
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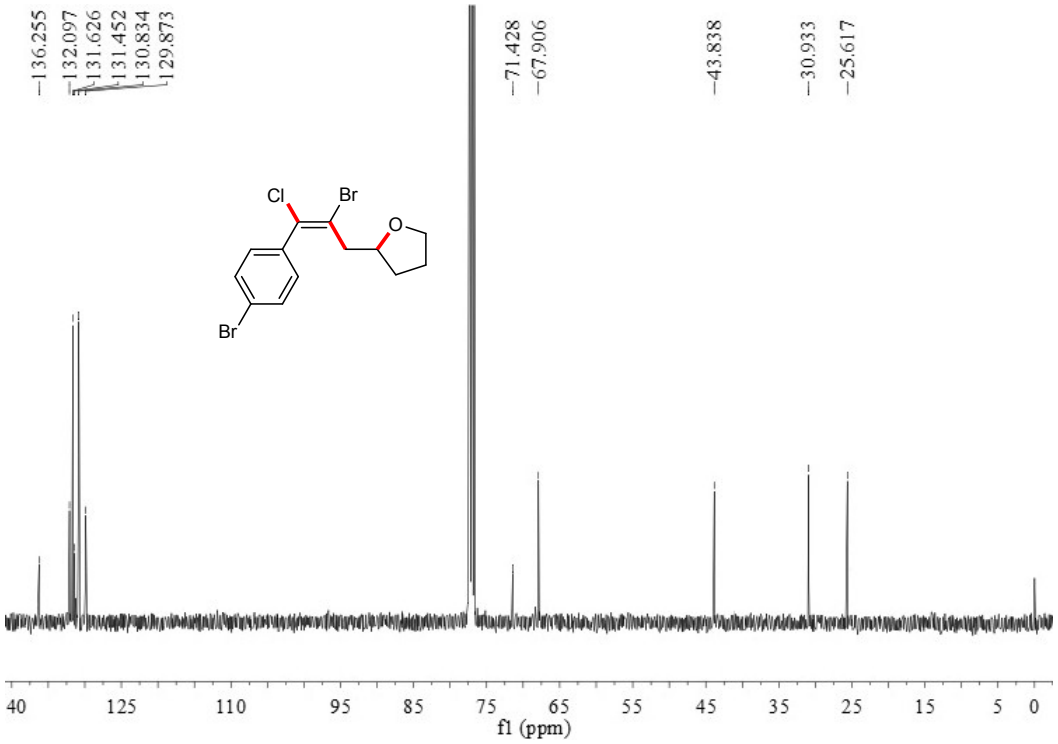
f1 (ppm)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67.906
43.838
30.933
25.617
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O
Br
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125
110
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85
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65
55
45
35
25
15
5
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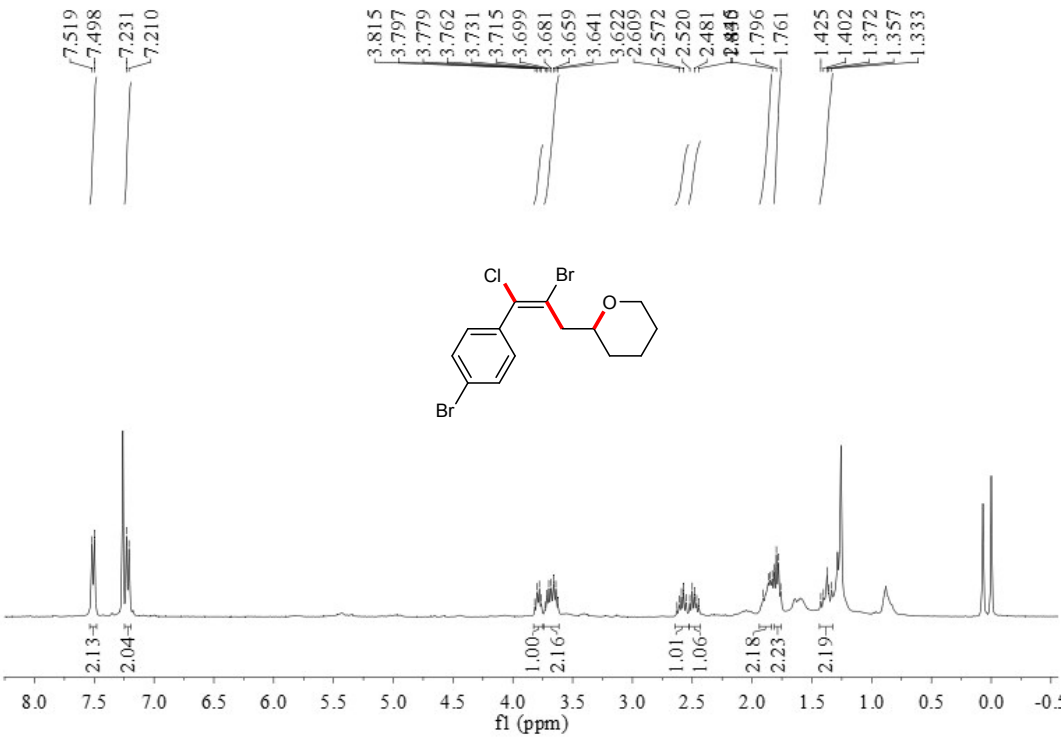
f1 (ppm)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3.762
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3.715
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3.681
3.659
3.641
3.622
2.609
2.572
2.520
2.481
1.796
1.761
1.425
1.402
1.372
1.357
1.333
Cl
Br
O
Br
2.13
2.04
1.00
2.16
1.01
1.06
2.18
2.23
2.19
8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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2.5
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1.0
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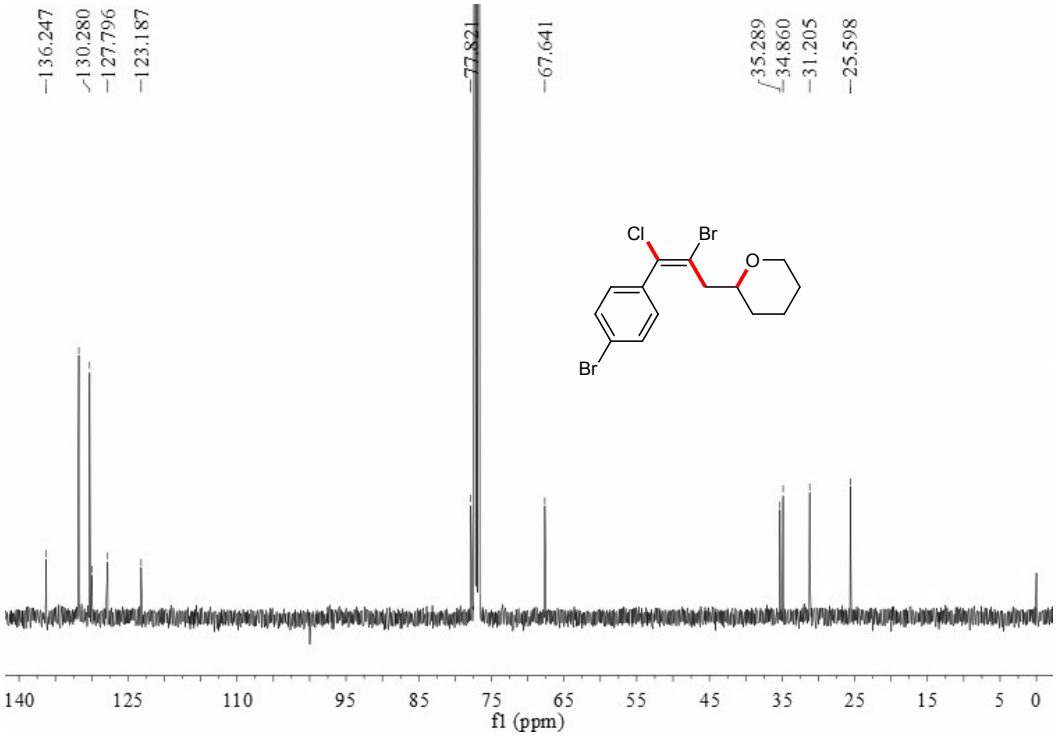
f1 (ppm)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67.641
35.289
34.860
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25.598
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Br
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125
110
95
85
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65
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45
35
25
15
5
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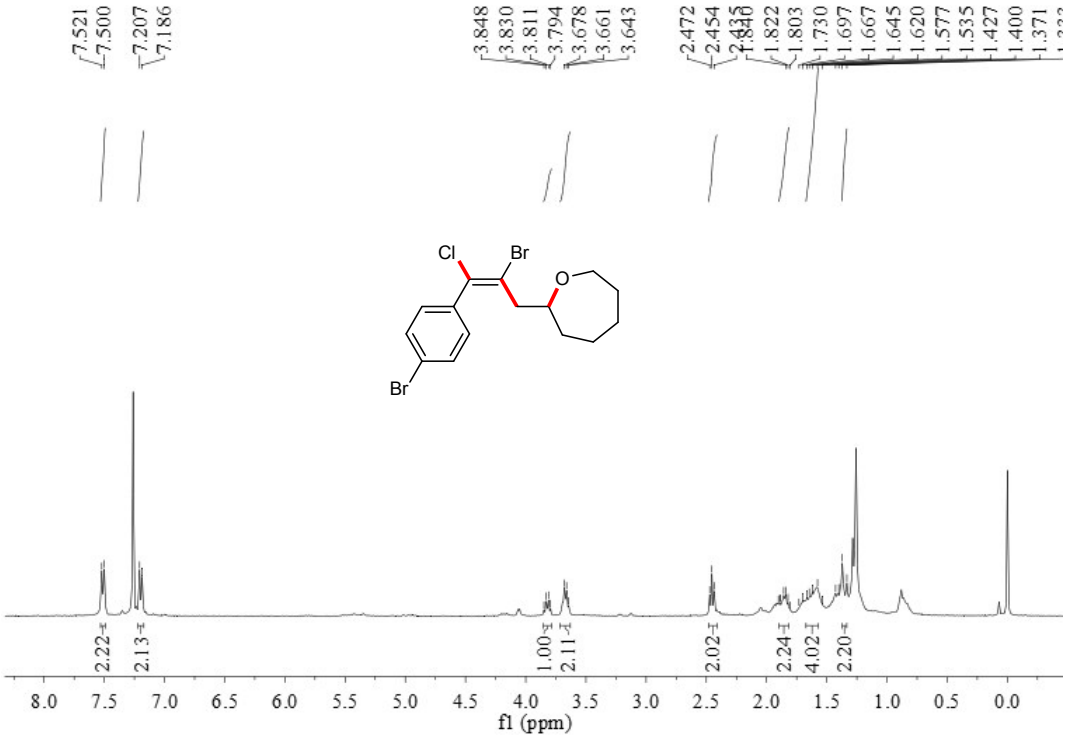
f1 (ppm)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1.822
1.803
1.730
1.697
1.667
1.645
1.620
1.577
1.535
1.427
1.400
1.371
Cl
Br
O
Br
2.22
2.13
1.00
2.11
2.02
2.24
4.02
2.20
8.0
7.5
7.0
6.5
6.0
5.5
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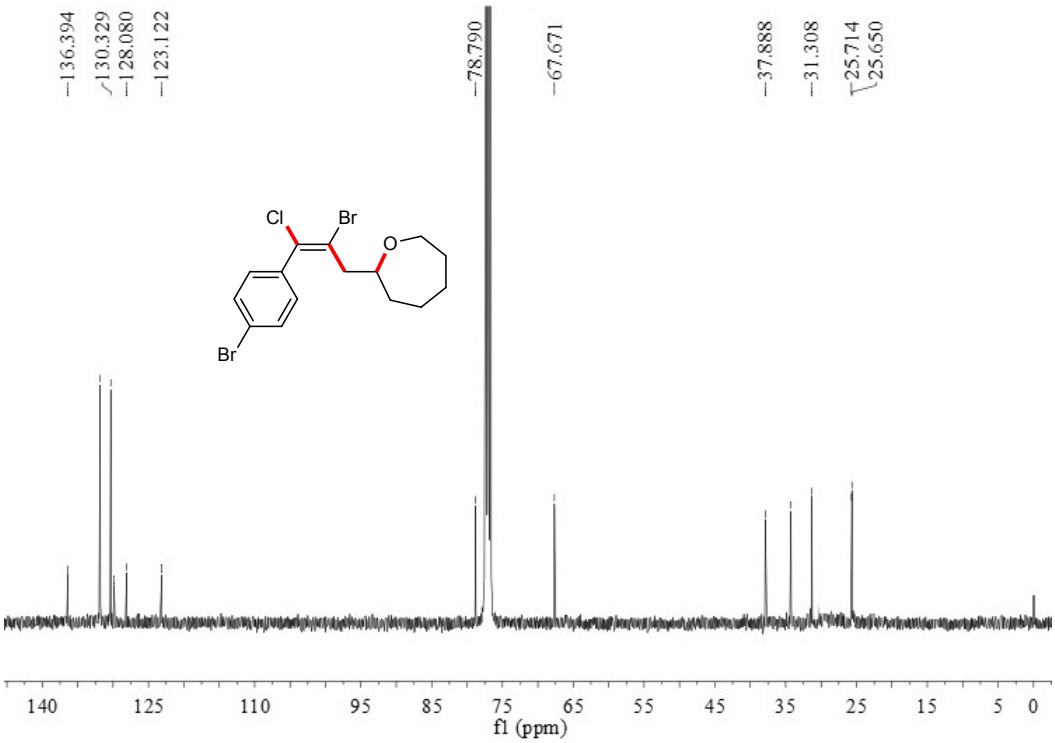
f1 (ppm)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130.329
128.080
123.122
78.790
67.671
37.888
31.308
25.714
25.650
Cl
Br
O
Br
140
125
110
95
85
75
65
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45
35
25
15
5
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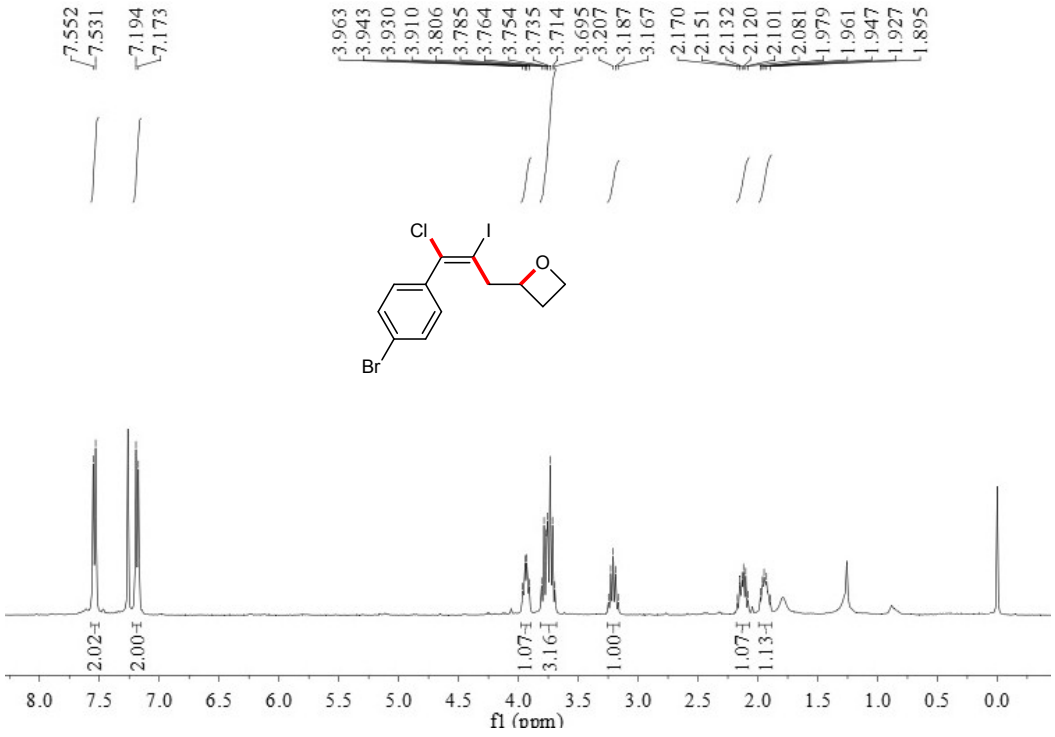
f1 (ppm)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3.735
3.714
3.695
3.207
3.187
3.167
2.170
2.151
2.132
2.120
2.101
2.081
1.979
1.961
1.947
1.927
1.895
Cl
I
O
Br
2.02
2.00
1.07
3.16
1.00
1.07
1.13
8.0
7.5
7.0
6.5
6.0
5.5
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2.5
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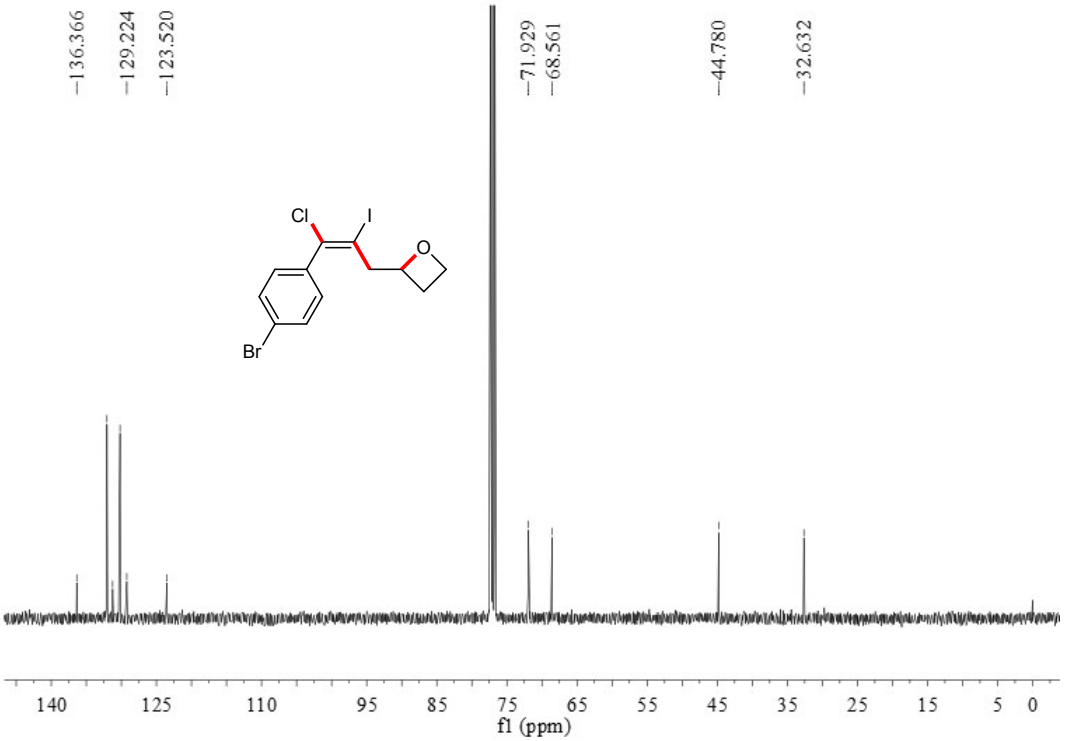
f1 (ppm)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O
Br
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125
110
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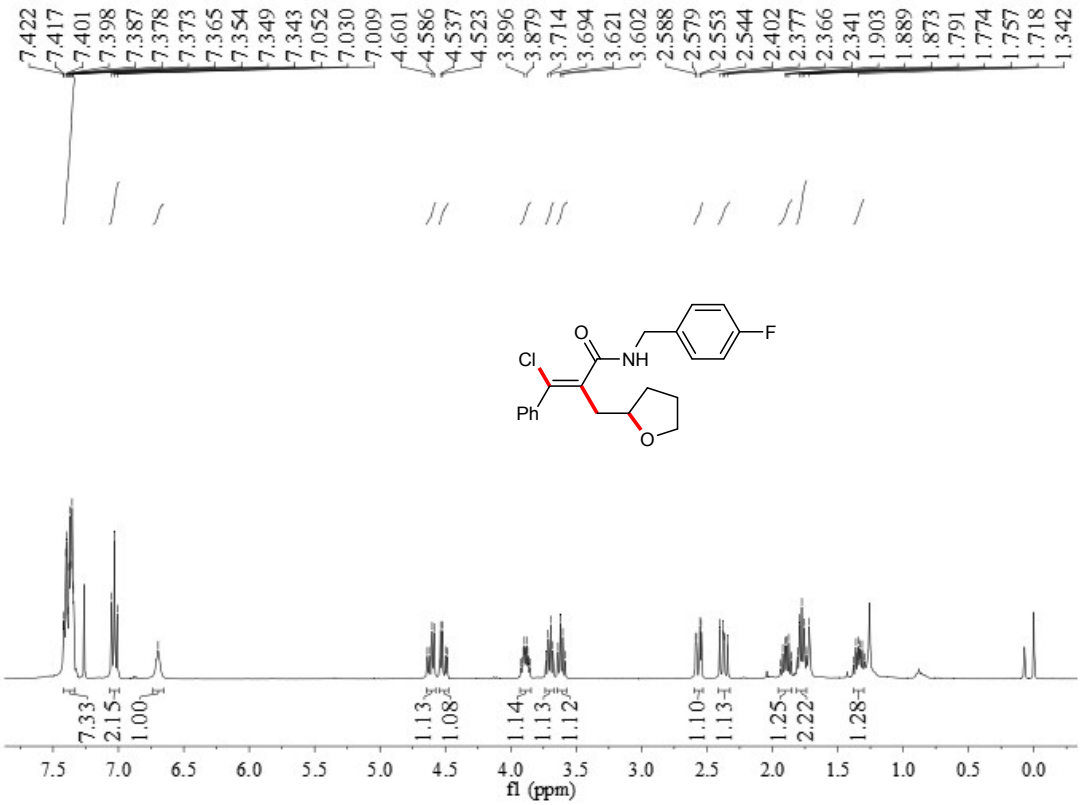
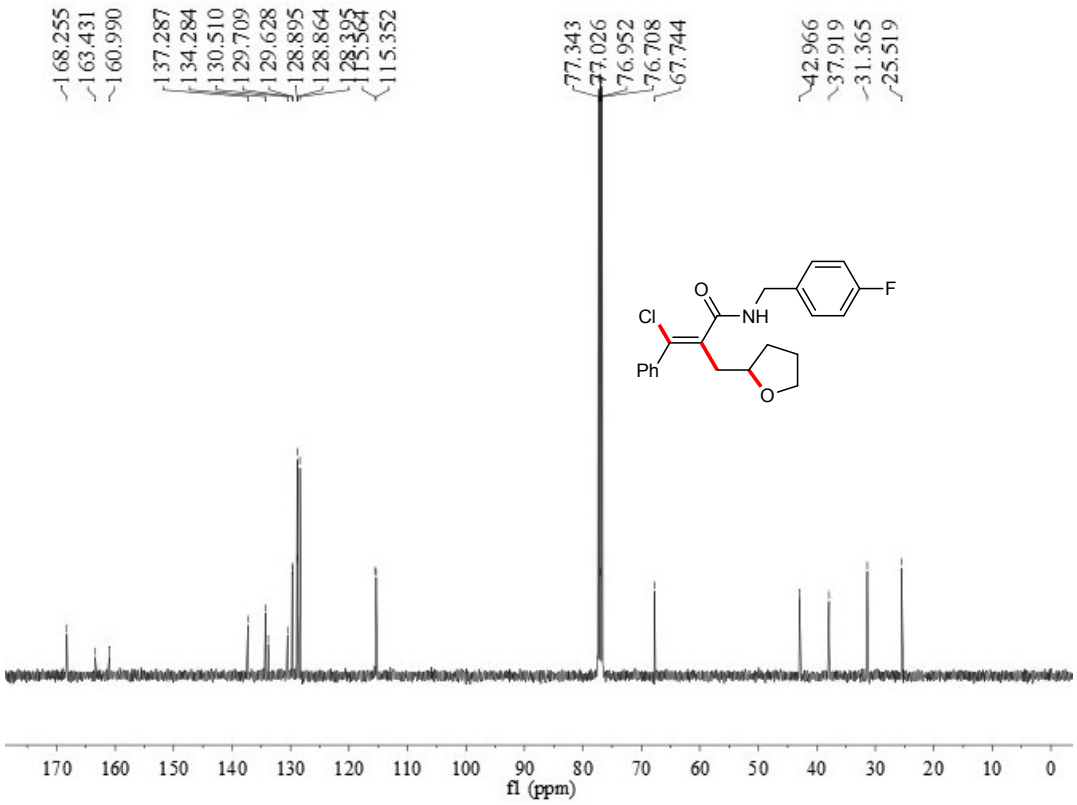
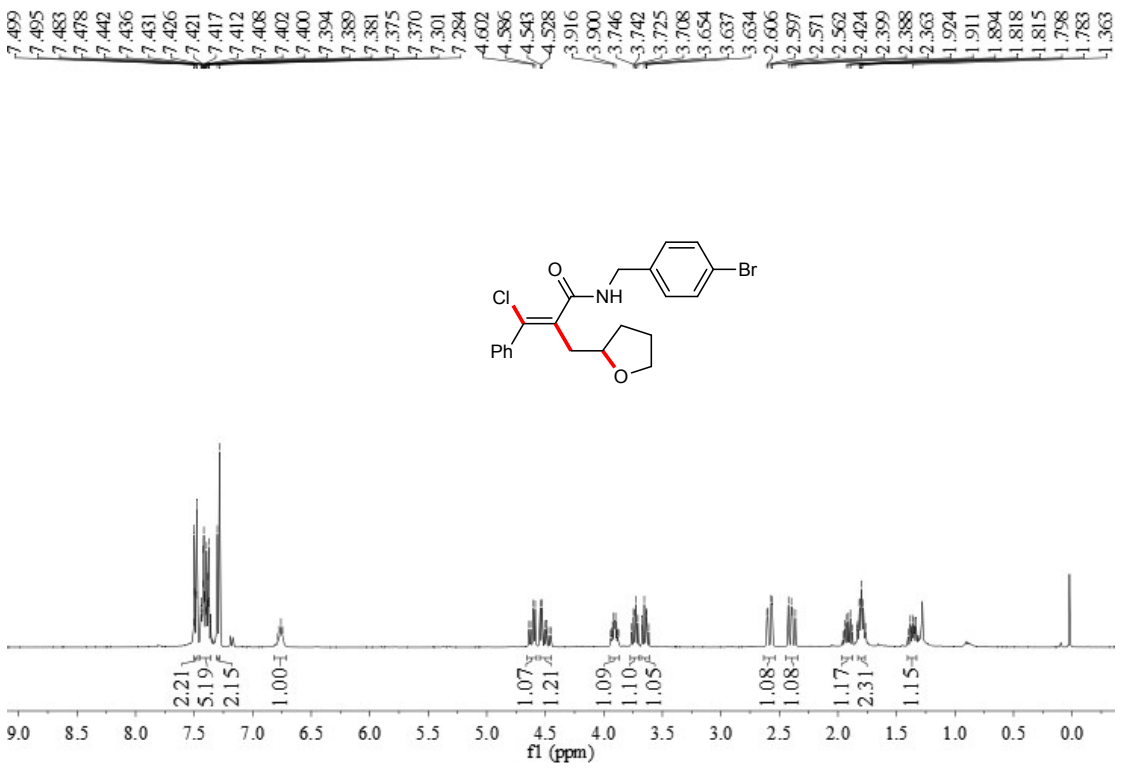
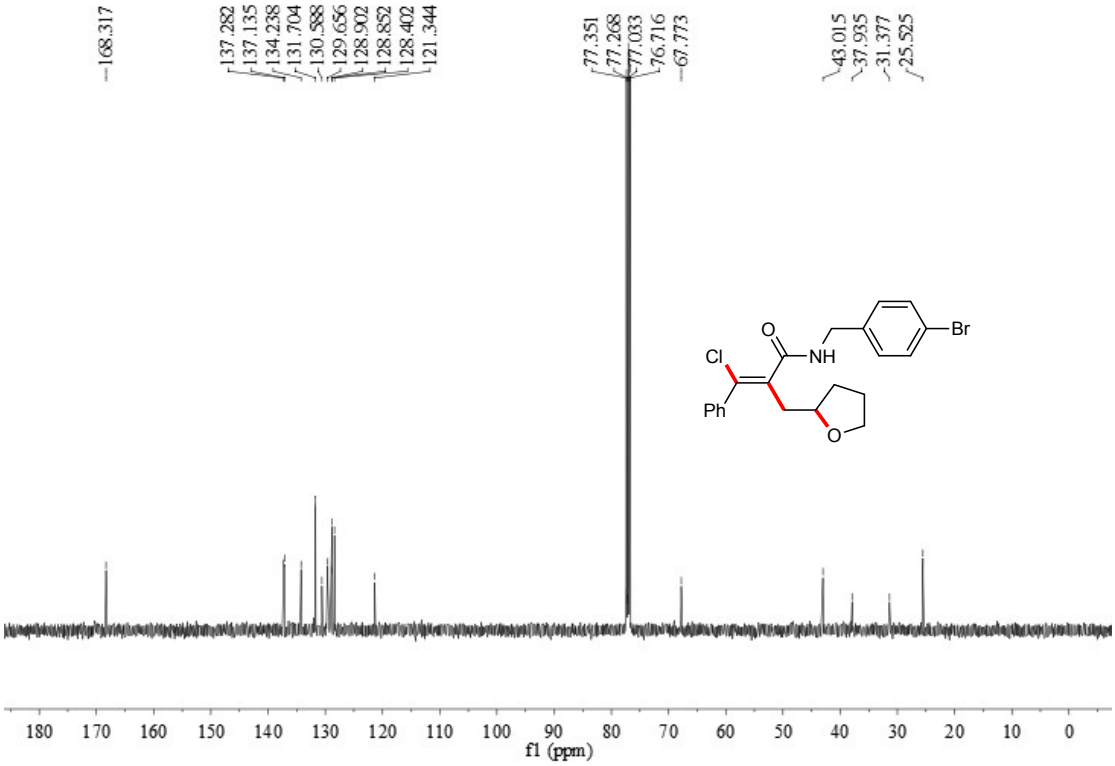
85
75
65
55
45
35
25
15
5
0
f1 (ppm)


7.422
7.417
7.401
7.398
7.387
7.378
7.373
7.365
7.354
7.349
7.343
7.052
7.030
7.009
4.601
4.586
4.537
4.523
3.896
3.879
3.714
3.694
3.621
3.602
2.588
2.579
2.553
2.544
2.402
2.377
2.366
2.341
1.903
1.889
1.873
1.791
1.774
1.757
1.718
1.342
O
NH
F
Cl
Ph
O
7.33
2.15
1.00
1.13
1.08
1.14
1.13
1.12
1.10
1.13
1.25
2.22
1.28
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


168.255
163.431
160.990
137.287
134.284
130.510
129.709
129.628
128.895
128.864
115.564
115.352
77.343
77.026
76.952
76.708
67.744
42.966
37.919
31.365
25.519
O
NH
F
Cl
Ph
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.499
7.495
7.483
7.478
7.442
7.436
7.431
7.426
7.421
7.417
7.412
7.408
7.402
7.400
7.394
7.389
7.381
7.375
7.370
7.301
7.284
4.602
4.586
4.543
4.528
3.916
3.900
3.746
3.742
3.725
3.708
3.654
3.637
3.634
2.606
2.597
2.571
2.562
2.424
2.399
2.388
2.363
1.924
1.911
1.894
1.818
1.815
1.798
1.783
1.363
O
NH
Br
Cl
Ph
O
2.21
5.19
2.15
1.00
1.07
1.21
1.09
1.10
1.05
1.08
1.08
1.17
2.31
1.15
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



Studies on the Stereochemistry of 3a